-1-

CAR LIGAND-BINDING DOMAIN POLYPEPTIDE CO-CRYSTALLIZED WITH A LIGAND, AND METHODS OF DESIGNING LIGANDS THAT MODULATE CAR ACTIVITY

5 <u>Technical Field</u>

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The present invention relates generally to the structure of the ligand-binding domain of CAR, and more particularly to the structure of the ligand-binding domain of CAR in complex with a ligand. The present invention also relates to CAR binding compounds and to the design of compounds that bind to CAR.

Abbreviations

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15	amu	-	atomic mass unit(s)
	ATP	-	adenosine triphosphate
	ADP	-	adenosine diphosphate
	BSA	-	bovine serum albumin
	CaMV	•	cauliflower mosaic virus
20	CAR	-	constitutive androstane receptor
	CARa	-	constitutive androstane receptor alpha
	CBP	-	CREB binding protein
	CCDB	-	Cambridge Crystallographic Data Bank
	cDNA	-	complementary DNA
25	CPU	-	central processing unit
	RAM	-	random access memory
	CRT	-	cathode-ray tube
	DBD	-	DNA binding domain
	DMSO	-	dimethyl sulfoxide
30	DNA	-	deoxyribonucleic acid
	DTT	-	dithiothreitol
	EDTA	-	ethylenediaminetetraacetic acid
	Et ₂ O	-	diethyl ether
	FEDs		field emission displays

-2-

	GST	-	glutathione S-transferase
	HEPES	-	N-2-hydroxyethylpiperazine-N'-2-
			ethanesulfonic acid
	kDa	-	kilodalton(s)
5	LBD	-	ligand-binding domain
	LCDs	-	liquid crystal displays
	LED	-	light emitting diode
	MPD	-	methyl-pentanediol
	MCAR	-	mouse constitutive androstane receptor
10	MIR	-	multiple isomorphous replacement
	MPD	-	methyl pentanediol
	N-COR	-	nuclear co-repressor
	NDP	-	nucleotide diphosphate
	NR	-	nuclear receptor
15	nt	-	nucleotide(s)
	NTP	-	nucleotide triphosphate
	PAGE	-	polyacrylamide gel electrophoresis
	PCR	-	polymerase chain reaction
	PEG	-	polyethylene glycol
20	pl	-	isoelectric point
	PXR	-	pregnane X receptor
	PBREM	-	phenobarbital-responsive enhancer module
	RAR	-	retinoic acid receptor
	RAREs	-	retinoic acid response elements
25	rCAR	-	rat constitutive androstane receptor
	RUBISCO	-	ribulose bisphosphate carboxylase
	RXR	-	retinoid X receptor
	SDS	-	sodium dodecyl sulfate
	SDS-PAGE	-	sodium dodecyl sulfate polyacrylamide gel
30			electrophoresis
	SMRT	-	silencing mediator for retinoid and thyroid
			receptors

-3-

SRC-1 - steroid receptor coactivator-1
SR - steroid receptor
TFA - trifluoroacetic acid
TMV - tobacco mosaic virus
TR - thyroid receptor
VDR - vitamin D receptor

Amino Acid Abbreviations, Codes, and Functionally Equivalent Codons

	Amino Acid	3-Letter	1-Letter	Codons
10	Alanine	Ala	Α	GCA GCC GCG GCU
	Arginine	Arg	R	AGA AGG CGA CGC CGG CGU
	Asparagine	Asn	N	AAC AAU
	Aspartic Acid	Asp	D	GAC GAU
	Cysteine	Cys	С	UGC UGU
15	Glutamic acid	Glu	E	GAA GAG
	Glutamine	Gln	Q	CAA CAG
	Glycine	Gly	G	GGA GGC GGG GGU
	Histidine	His	Н	CAC CAU
	Isoleucine	lle	1	AUA AUC AUU
20	Leucine	Leu	L	UUA UUG CUA CUC CUG CUU
	Lysine	Lys	K	AAA AAG
	Methionine	Met	M	AUG
	Phenylalanine	Phe	F	UUC UUU
	Proline	Pro	Р	CCA CCC CCG CCU
25	Serine	Ser	S	ACG AGU UCA UCC UCG UCU
	Threonine	Thr	Т	ACA ACC ACG ACU
	Tryptophan	Trp	W	UGG
	Tyrosine	Tyr	Y	UAC UAU
	Valine	Val	V	GUA GUC GUG GUU
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-4-

Background

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The constitutive androstane receptor (CAR; Unified Nomenclature Committee designation NR1I3) was isolated in 1994 by screening a human liver library with a degenerate oligonucleotide probe based on the P box region (Baes et al., 1994). CAR was subsequently shown to be a heterodimer partner for RXR that acts as a specific, retinoid-independent activator of a subset of retinoic acid response elements (RAREs). The mouse CAR homologue was also isolated in 1994 (Honkakoski et al., 1998). Mouse CAR studies showed that RXR and CAR bind to a site in the phenobarbital-responsive enhancer module (PBREM) of the cytochrome P-450 Cyp2b10 gene in response to phenobarbital induction. Expression of RXR and CAR in mammalian cell lines activated PBREM, indicating that a CAR-RXR heterodimer is a trans-acting factor for the mouse Cyp2b10 gene. These studies were the first to indicate that CAR might play a role in response to xenobiotics.

The ability to respond to a wide range of potentially toxic chemicals is essential in a complex environment. Evidence is accumulating that CAR and its closest mammalian homologue, the pregnane X receptor (PXR; Unified Nomenclature Committee designation NR1I2), evolved to detect xenobiotics as part of the body's detoxification machinery (Waxman, 1999). Both receptors are highly expressed in the liver and intestine and both regulate the expression of specific detoxification genes. PXR and CAR regulate genes whose protein products are involved in the hydroxylation (phase I), conjugation (phase II), and transport of xenobiotics (phase III). CAR is activated by some of the same ligands as PXR (Moore et al., 2000), regulates at least partially overlapping sets of genes (e.g. CYP3A and CYP2B; Xie et al., 2000a), and can signal through the same response elements (Goodwin et al., 2001; Handschin et al., 2001).

Despite these similarities, CAR differs from PXR in several respects. CAR ligand binding has been shown to be more restricted than that of PXR (Moore *et al.*, 2000). Furthermore, CAR displays a high basal level of activity relative to PXR that can be reduced by the binding of either naturally

-5-

occurring androstanes or xenobiotics such as clotrimazole (Baes et al., 1994; Moore et al., 2000). Finally, CAR displays fundamental differences from PXR with regard to its cellular regulation. In mouse primary hepatocytes and in mouse liver in vivo, CAR is cytoplasmic in the naïve state and translocates to the nucleus upon activation (Kawamoto et al., 1999), a process thought to be regulated in part by dephosphorylation of the receptor (Honkakoski et al., 1998). Induction of CAR nuclear translocation does not necessarily depend upon ligand-binding, as phenobarbital has been shown to be an activator of CAR in vivo and in hepatocytes, but does not appear to interact directly with the CAR ligand-binding domain (Moore et al., 2000). Thus, CAR has a high basal level of transcriptional activity even in the absence of an exogenous ligand. An important goal of future efforts will be to further differentiate the physical and functional properties of CAR from PXR, and to ultimately distinguish the unique physiological role of CAR.

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Towards this goal, the CAR gene has recently been "knocked-out" by targeted gene disruption (Xie et al., 2000b). The loss of CAR expression did not result in any overt phenotype. Homozygous CAR-1- animals were born at the expected Mendelian frequency, and both male and female CAR-deficient animals were fertile. It was further demonstrated that the nuclear receptor CAR mediates the Cyp2b10 gene response evoked by phenobarbital-like inducers, as well as by the more potent TCPOBOP compound (Xie et al., 2000b). When challenged, these animals showed decreased metabolism of the classic CYP substrate zoxazolamine and a complete loss of the liver hypertrophic and hyperplastic responses to these compounds. These experiments were thus consistent with the notion that at least one aspect of the physiological role of CAR involves xenobiotic metabolism.

Further insight into CAR is expected to be gleaned from CAR structural studies. The availability of the CAR structure will allow an understanding of ligand modulation of CAR activity and will facilitate the design of novel CAR ligands. The present invention addresses these and other needs in the art.

-6-

Summary of the Invention

The present invention provides a crystalline form comprising a substantially pure constitutive androstane receptor (CAR) ligand-binding domain polypeptide. In one embodiment, the crystalline form comprises a substantially pure constitutive androstane receptor (CAR) ligand-binding domain polypeptide in complex with a ligand. In one embodiment, a ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide.

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The present invention also provides a method of generating a crystalline form comprising a constitutive androstane receptor (CAR) ligand-binding domain polypeptide in complex with a ligand, the method comprising: (a) incubating a solution comprising a constitutive androstane receptor (CAR) ligand-binding domain and a ligand with an equal volume of reservoir; and (b) crystallizing the constitutive androstane receptor (CAR) ligand-binding domain polypeptide and ligand using the hanging drop method, whereby a crystalline form of a constitutive androstane receptor (CAR) ligand-binding domain polypeptide in complex with a ligand is generated. Also provided is a crystalline form formed by the above-recited method. In one embodiment, a ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide.

The present invention also provides a method of designing a chemical compound that modulates the biological activity of a target constitutive androstane receptor (CAR) polypeptide. In one embodiment, the method comprises: obtaining one or more three-dimensional structures for the ligand-binding domain (LBD) of constitutive androstane receptor (CAR) in a repressed conformation, and one or more three-dimensional structures of the LBD of constitutive androstane receptor (CAR) in an activated conformation; rotating and translating the three-dimensional structures as rigid bodies so as to superimpose corresponding backbone atoms of a core region of the constitutive androstane receptor (CAR) LBD; comparing one or both of: (i) the superimposed three-dimensional structures to identify volume near the ligand-binding pocket of the constitutive androstane receptor (CAR) LBD that is available to a ligand in the one or more activated structures, or in one or more

-7-

repressed structures, but that is not available to the ligand in one or more structures of the opposite class; and (ii) the superimposed three-dimensional structures to identify interactions that a ligand could make in one or more of the activated structures, or in one or more of the repressed structures, but which the ligand could not make in one or more structures of the opposite class; and designing a chemical compound that occupies the volume, makes the interaction, or both occupies the volume and makes the interaction.

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Optionally the method further comprises synthesizing the designed chemical compound; and testing the designed chemical compound in a biological assay to determine whether it acts as a ligand of constitutive androstane receptor (CAR) with an effect on constitutive androstane receptor (CAR) biological activities, whereby a ligand of a constitutive androstane receptor (CAR) polypeptide is designed.

In another embodiment, the volume or interaction is available in one or more of the repressed structures of constitutive androstane receptor (CAR), but not available in one or more of the activated structures of constitutive androstane receptor (CAR). In another embodiment, the method further comprises designing a chemical compound that promotes the binding of corepressor to the constitutive androstane receptor (CAR) LBD by making direct favorable interactions with the co-repressor. In another embodiment, the method further comprises designing a chemical compound that reduces binding of a co-repressor to the constitutive androstane receptor (CAR) LBD by making direct unfavorable interactions with the co-repressor. In another embodiment, the method further comprises designing a chemical compound that promotes coactivator binding by displacing an AF2 helix of the constitutive androstane receptor (CAR) LBD and making direct favorable interactions with a coactivator, where the designing allows for an expected movement of the coactivator within a coactivator/co-repressor binding pocket. In yet another embodiment, the method further comprises designing a chemical compound by considering a known agonist of the constitutive androstane receptor (CAR) and adding a substituent that protrudes into the volume identified in step (c) or that makes a desired interaction.

-8-

The present invention also provides a binding site in a human constitutive androstane receptor (CAR) polypeptide for a constitutive androstane receptor ligand, wherein the ligand is in van der Waals, hydrogen binding, or van der Waals and hydrogen binding contact with at least one residue of the human constitutive androstane receptor polypeptide.

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The present invention also provides a complex of a human constitutive androstane receptor (CAR) ligand-binding domain and a ligand, wherein the ligand is in van der Waals, hydrogen bonding, or both van der Waals and hydrogen bonding contact with at least one of the following residues of the human constitutive androstane receptor polypeptide: Phe161, Ile164, Asn165, Val199, His203, Phe217, Trp224, Thr225, Ile226, Asp228, Gly229, Gln234, Phe238, Leu239, Leu242, Phe243, Tyr326, Met339, Met340.

The present invention also provides a crystal of a complex of a human constitutive androstane receptor (CAR) ligand-binding domain and a ligand, wherein the ligand is in van der Waals, hydrogen bonding, or both van der Waals and hydrogen bonding contact with at least one of the following residues of the human constitutive androstane receptor polypeptide: Phe161, lle164, Asn165, Val199, His203, Phe217, Trp224, Thr225, lle226, Asp228, Gly229, Gln234, Phe238, Leu239, Leu242, Phe243, Tyr326, Met339, Met340. In one embodiment, the constitutive androstane receptor is a human constitutive androstane receptor and the crystal has the following physical measurements: space group P2₁2₁2₁, and unit cell: $\alpha = 83.0$ angstroms, $\alpha = 83.0$ angstroms, and $\alpha = 83.0$ angstroms.

The present invention also provides a method for designing a ligand of a constitutive androstane receptor (CAR) polypeptide, the method comprising: (a) forming a complex of a compound bound to the constitutive androstane receptor (CAR) polypeptide; (b) determining a structural feature of the complex formed in (a); wherein the structural feature is of a binding site for the compound; and (c) using the structural feature determined in (b) to design a ligand of a constitutive androstane receptor (CAR) polypeptide capable of binding to the binding site of the present invention. In one embodiment, the

-9-

method of the present invention further comprises using a computer-based model of the complex formed in (a) in designing the ligand.

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The present invention also provides a method of designing a ligand that selectively modulates the activity of a constitutive androstane receptor (CAR) polypeptide, the method comprising: (a) evaluating a three-dimensional structure of a crystallized constitutive androstane receptor (CAR) ligandbinding domain polypeptide in complex with a ligand; and (b) synthesizing a potential ligand based on the three-dimensional structure of the crystallized constitutive androstane receptor (CAR) catalytic polypeptide in complex with a ligand, whereby a ligand that selectively modulates the activity of a constitutive androstane receptor (CAR) polypeptide is designed. In one embodiment, the constitutive androstane receptor (CAR) ligand-binding domain polypeptide comprises the amino acid sequence of SEQ ID NO: 4. In one embodiment, the crystalline form is such that the three-dimensional structure of the crystallized constitutive androstane receptor (CAR) ligandbinding domain polypeptide in complex with a ligand can be determined to a resolution of about 2.15 Å or better. In one embodiment, the method further comprises contacting a constitutive androstane receptor (CAR) ligand-binding domain polypeptide with the potential ligand and a ligand; and assaying the constitutive androstane receptor (CAR) ligand-binding domain polypeptide for binding of the potential ligand, for a change in activity of the constitutive androstane receptor (CAR) ligand-binding domain polypeptide, or both. In one embodiment, the ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1Hbenzimidazole-6-carboxamide.

The present invention also provides a method of screening a plurality of compounds for a ligand of a constitutive androstane receptor (CAR) ligand-binding domain polypeptide, the method comprising: (a) providing a library of test samples; (b) contacting a crystalline form comprising a constitutive androstane receptor (CAR) polypeptide in complex with a ligand with each test sample; (c) detecting an interaction between a test sample and the crystalline constitutive androstane receptor (CAR) polypeptide in complex with a ligand; (d) identifying a test sample that interacts with the crystalline

-10-

constitutive androstane receptor (CAR) polypeptide in complex with a ligand; and (e) isolating a test sample that interacts with the crystalline constitutive androstane receptor (CAR) polypeptide in complex with a ligand, whereby a plurality of compounds is screened for a ligand of a constitutive androstane receptor (CAR) ligand-binding domain polypeptide. In one embodiment, the CAR polypeptide comprises a CAR ligand-binding domain. In another embodiment, the CAR polypeptide is a human CAR polypeptide. In yet another embodiment, the CAR polypeptide comprises the amino acid sequence of SEQ ID NO: 4. In one embodiment, the library of test samples is bound to a substrate. In another embodiment, the library of test samples is synthesized directly on a substrate. In one embodiment, the ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide,

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The present invention also provides a method for identifying a constitutive androstane receptor (CAR) ligand, the method comprising: (a) providing atomic coordinates of a constitutive androstane receptor (CAR) ligand-binding domain in complex with a ligand to a computerized modeling system; and (b) modeling a ligand that fits spatially into the binding pocket of the constitutive androstane receptor (CAR) ligand-binding domain to thereby identify a constitutive androstane receptor (CAR) ligand. In one embodiment, the method further comprises identifying in an assay for constitutive androstane receptor (CAR)-mediated activity a modeled ligand that increases or decreases the activity of the constitutive androstane receptor (CAR). In one embodiment, the CAR is a human CAR. In one embodiment, the CAR ligand-binding domain comprises the amino acid sequence of SEQ ID NO: 4. In one embodiment, the ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide.

The present invention also provides a method of identifying a constitutive androstane receptor (CAR) ligand that selectively binds a constitutive androstane receptor (CAR) polypeptide compared to other polypeptides, the method comprising: (a) providing atomic coordinates of a constitutive androstane receptor (CAR) ligand-binding domain in complex with a ligand to a computerized modeling system; and (b) modeling a ligand that

-11-

fits into the binding pocket of a constitutive androstane receptor (CAR) ligand-binding domain and that interacts with residues of a constitutive androstane receptor (CAR) ligand-binding domain that are conserved among constitutive androstane receptor (CAR) subtypes to thereby identify a constitutive androstane receptor (CAR) ligand that selectively binds a constitutive androstane receptor (CAR) polypeptide compared to other polypeptides. In one embodiment, the method further comprises identifying in a biological assay for constitutive androstane receptor (CAR) activity a modeled ligand that selectively binds to said constitutive androstane receptor (CAR) and increases or decreases the activity of the constitutive androstane receptor (CAR). In one embodiment, the CAR ligand-binding domain comprises the amino acid sequence shown in SEQ ID NO: 4. In one embodiment, the ligand is 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide.

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The present invention also provides a method of designing a ligand of a constitutive androstane receptor (CAR) polypeptide, the method comprising: (a) selecting a candidate constitutive androstane receptor (CAR) ligand; (b) determining which amino acid or amino acids of a constitutive androstane receptor (CAR) polypeptide interact with the ligand using a three-dimensional model of a crystallized protein, the model comprising a constitutive androstane receptor (CAR) ligand-binding domain in complex with a ligand; (c) identifying in a biological assay for constitutive androstane receptor (CAR) activity a degree to which the ligand modulates the activity of the constitutive androstane receptor (CAR) polypeptide; (d) selecting a chemical modification of the ligand wherein the interaction between the amino acids of the constitutive androstane receptor (CAR) polypeptide and the ligand is predicted to be modulated by the chemical modification; (e) synthesizing a ligand having the chemical modified to form a modified ligand; (f) contacting the modified ligand with the constitutive androstane receptor (CAR) polypeptide; (g) identifying in a biological assay for constitutive androstane receptor (CAR) activity a degree to which the modified ligand modulates the biological activity of the constitutive androstane receptor (CAR) polypeptide; and (h) comparing the biological activity of the constitutive androstane

-12-

receptor (CAR) polypeptide in the presence of modified ligand with the biological activity of the constitutive androstane receptor (CAR) polypeptide in the presence of the unmodified ligand, whereby a ligand of a constitutive androstane receptor (CAR) polypeptide is designed. In one embodiment, wherein the method further comprises repeating steps (a) through (f), if the biological activity of the constitutive androstane receptor (CAR) polypeptide in the presence of the modified ligand varies from the biological activity of the constitutive androstane receptor (CAR) polypeptide in the presence of the unmodified ligand.

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The present invention also provides a crystallized, recombinant polypeptide comprising: (a) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (b) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (c) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of constitutive androstane receptor (CAR); wherein the polypeptide of (a), (b) or (c) is in crystal form. In one embodiment, the crystallized, recombinant polypeptide diffracts X-rays to a resolution of about 2.5 Å or better. In another embodiment, the polypeptide is labeled with seleno-methionine.

The present invention also provides a method for designing a modulator for the prevention or treatment of a disease or disorder, comprising:

(a) providing a three-dimensional structure for a crystallized, recombinant polypeptide; (b) identifying a potential modulator for the prevention or treatment of a disease or disorder by reference to the three-dimensional structure; (c) contacting a polypeptide or a constitutive androstane receptor (CAR) with the potential modulator; and (d) assaying the activity of the polypeptide after contact with the modulator, wherein a change in the activity of the polypeptide indicates that the modulator can be useful for prevention or treatment of a disease or disorder.

The present invention also provides a method for obtaining structural information of a crystallized polypeptide, the method comprising: (a) crystallizing a recombinant polypeptide, wherein the polypeptide comprises: (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); and wherein the crystallized polypeptide is capable of diffracting X-rays to a resolution of 2.5 Å or better; and (b) analyzing the crystallized polypeptide by X-ray diffraction to determine the three-dimensional structure of at least a portion of the crystallized In one embodiment, the three-dimensional structure of the polypeptide. portion of the crystallized polypeptide is determined to a resolution of 2.5 Å or better.

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The present invention also provides a method for identifying a druggable region of a polypeptide, the method comprising: (a) obtaining crystals of a polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR), such that the three dimensional structure of the crystallized polypeptide can be determined to a resolution of 2.5 Å or better; (b) determining the three dimensional structure of the crystallized polypeptide using X-ray diffraction; and (c) identifying a druggable region of the crystallized polypeptide based on the three-dimensional structure of the crystallized polypeptide. embodiment, the druggable region is an active site. In another embodiment, the druggable region is on the surface of the polypeptide.

-14-

The present invention also provides a crystalline human constitutive androstane receptor (CAR) comprising a crystal having unit cell dimensions a = 83.0 Å; b = 116.8 Å; c = 131.9 Å; $\alpha = \beta = \gamma = 90^{\circ}$; with an orthorhombic space group P2₁2₁2₁ and 4 molecules per asymmetric unit.

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The present invention also provides a crystallized polypeptide comprising: (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); wherein the crystal has a P2₁2₁2₁ space group.

The present invention also provides a crystallized polypeptide comprising a structure of a polypeptide that is defined by a substantial portion of the atomic coordinates set forth in Table 2 or Table 3.

The present invention also provides a method for determining the crystal structure of a homolog of a polypeptide, the method comprising: (a) providing the three dimensional structure of a first crystallized polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); (b) obtaining crystals of a second polypeptide comprising an amino acid sequence that is at least 70% identical to the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4, such that the three dimensional structure of the second crystallized polypeptide can be determined to a resolution of 2.5 Å or better; and (c) determining the three dimensional structure of the second crystallized polypeptide by X-ray crystallography based on the atomic coordinates of the

-15-

three dimensional structure provided in step (a). In one embodiment, the atomic coordinates for the second crystallized polypeptide have a root mean square deviation from the backbone atoms of the first polypeptide of not more than 1.5 Å for all backbone atoms shared in common with the first polypeptide and the second polypeptide.

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The present invention also provides a method for homology modeling a homolog of human constitutive androstane receptor (CAR), comprising: (a) aligning the amino acid sequence of a homolog of human constitutive androstane receptor (CAR) with an amino acid sequence of SEQ ID NO: 2 or SEQ ID NO: 4 and incorporating the sequence of the homolog of human CAR into a model of human constitutive androstane receptor (CAR) derived from structure coordinates as listed in Table 2 or Table 3 to yield a preliminary model of the homolog of human CAR; (b) subjecting the preliminary model to energy minimization to yield an energy minimized model; (c) remodeling regions of the energy minimized model where stereochemistry restraints are violated to yield a final model of the homolog of human constitutive androstane receptor (CAR).

The present invention also provides a method for obtaining structural information about a molecule or a molecular complex of unknown structure comprising: (a) crystallizing the molecule or molecular complex; (b) generating an X-ray diffraction pattern from the crystallized molecule or molecular complex; (c) applying at least a portion of the structure coordinates set forth in Table 2 or Table 3 to the X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

The present invention also provides a method for attempting to make a crystallized complex comprising a polypeptide and a modulator having a molecular weight of less than 5 kDa, the method comprising: (a) crystallizing a polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that

-16-

hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); such that crystals of the crystallized polypeptide will diffract X-rays to a resolution of 5 Å or better; and (b) soaking the crystals in a solution comprising a potential modulator having a molecular weight of less than 5 kDa.

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The present invention also provides a method for incorporating a potential modulator in a crystal of a polypeptide, comprising placing a hexagonal crystal of human constitutive androstane receptor (CAR) having unit cell dimensions a = 83.0 Å; b = 116.8 Å; c = 131.9 Å, $a = b = g = 90^{\circ}$, with an orthorhombic space group P212121, in a solution comprising the potential modulator.

The present invention also provides a computer readable storage medium comprising digitally encoded structural data, wherein the data comprises structural coordinates as listed in Table 2 or Table 3 for the backbone atoms of at least about six amino acid residues from a druggable region of human constitutive androstane receptor (CAR).

The present invention also provides a scalable three-dimensional configuration of points, at least a portion of the points derived from some or all of the structure coordinates as listed in Table 2 or Table 3 for a plurality of amino acid residues from a druggable region of human constitutive androstane receptor (CAR). In one embodiment, the structure coordinates as listed in Table 2 or Table 3 for the backbone atoms of at least about five amino acid residues from a druggable region of human constitutive androstane receptor (CAR) are used to derive part or all of the portion of points. In another embodiment, the structure coordinates as listed in Table 2 or Table 3 for the backbone and optionally the side chain atoms of at least about ten amino acid residues from a druggable region of human constitutive androstane receptor (CAR) are used to derive part or all of the portion of points. In another embodiment, the structure coordinates as listed in Table 2 or Table 3 for the backbone atoms of at least about fifteen amino acid residues from a druggable region of human constitutive androstane receptor

(CAR) are used to derive part or all of the portion of points. In another embodiment, substantially all of the points are derived from structure coordinates as listed in Table 2 or Table 3. In still another embodiment, the structure coordinates as listed in Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR) are used to derive part or all of the portion of points.

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The present invention also provides a scalable three-dimensional configuration of points, comprising points having a root mean square deviation of less than about 1.5 Å from the three dimensional coordinates as listed in Table 2 or Table 3 for the backbone atoms of at least five amino acid residues, wherein the five amino acid residues are from a druggable region of human constitutive androstane receptor (CAR). In one embodiment, any point-to-point distance, calculated from the three dimensional coordinates as listed in Table 2 or Table 3, between one of the backbone atoms for one of the five amino acid residues and another backbone atom of a different one of the five amino acid residues is not more than about 10 Å.

The present invention also provides a scalable three-dimensional configuration of points comprising points having a root mean square deviation of less than about 1.5 Å from the three dimensional coordinates as listed in Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR).

The present invention also provides a computer readable storage medium comprising digitally encoded structural data, wherein the data comprise the identity and three-dimensional coordinates as listed in Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR).

The present invention also provides a scalable three-dimensional configuration of points, wherein the points have a root mean square deviation of less than about 1.5 Å from the three dimensional coordinates as listed in

-18-

Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR), wherein up to one amino acid residue in each of the regions can have a conservative substitution thereof.

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The present invention also provides a scalable three-dimensional configuration of points derived from a druggable region of a polypeptide, wherein the points have a root mean square deviation of less than about 1.5 Å from the three dimensional coordinates as listed in Table 2 or Table 3 for the backbone atoms of at least ten amino acid residues that participate in the intersubunit contacts of human constitutive androstane receptor (CAR).

The present invention also provides a computer-assisted method for identifying an inhibitor of the activity of human constitutive androstane receptor (CAR), comprising: (a) supplying a computer modeling application with a set of structure coordinates as listed in Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR) so as to define part or all of a molecule or complex; (b) supplying the computer modeling application with a set of structure coordinates of a chemical entity; and (c) determining whether the chemical entity is expected to bind to or interfere with the molecule or complex. In one embodiment, determining whether the chemical entity is expected to bind to or interfere with the molecule or complex comprises performing a fitting operation between the chemical entity and a druggable region of the molecule or complex, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the druggable region. In one embodiment, the method further comprises screening a library of chemical entities.

The present invention also provides a computer-assisted method for designing an inhibitor of constitutive androstane receptor (CAR) activity comprising: (a) supplying a computer modeling application with a set of structure coordinates having a root mean square deviation of less than about 1.5 Å from the structure coordinates as listed in Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable

regions of human constitutive androstane receptor (CAR) so as to define part or all of a molecule or complex; (b) supplying the computer modeling application with a set of structure coordinates for a chemical entity; (c) evaluating the potential binding interactions between the chemical entity and the molecule or complex; (d) structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and (e) determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of constitutive androstane receptor (CAR) activity. embodiment, determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or complex comprises performing a fitting operation between the chemical entity and the molecule or complex, followed by computationally analyzing the results of the fitting operation to evaluate the association between the chemical entity and the molecule or complex. In another embodiment, the set of structure coordinates for the chemical entity is obtained from a chemical library.

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The present invention also provides a computer-assisted method for designing an inhibitor of constitutive androstane receptor (CAR) activity de novo comprising: (a) supplying a computer modeling application with a set of three-dimensional coordinates derived from the structure coordinates as listed in Table 2 or Table 3 for the atoms of the amino acid residues from any of the above-described druggable regions of human constitutive androstane receptor (CAR) so as to define part or all of a molecule or complex; (b) computationally building a chemical entity represented by a set of structure coordinates; and (c) determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or complex, wherein binding to or interfering with the molecule or complex is indicative of potential inhibition of constitutive androstane receptor (CAR) activity. In one embodiment, determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or complex comprises performing a fitting operation between the chemical entity and a druggable region of the

-20-

molecule or complex, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the druggable region.

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The present invention also provides a method for identifying a potential modulator for the prevention or treatment of a disease or disorder, the method comprising: (a) providing the three dimensional structure of a crystallized polypeptide comprising: (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); (b) obtaining a potential modulator for the prevention or treatment of a disease or disorder based on the three dimensional structure of the crystallized polypeptide; (c) contacting the potential modulator with a second polypeptide comprising: (i) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (ii) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (iii) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); which second polypeptide can optionally be the same as the crystallized polypeptide; and (d) assaying the activity of the second polypeptide, wherein a change in the activity of the second polypeptide indicates that the compound can be useful for prevention or treatment of a disease or disorder.

The present invention also provides a method for designing a candidate modulator for screening for inhibitors of a polypeptide, the method comprising: (a) providing the three dimensional structure of a druggable region of a polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least

about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); and (b) designing a candidate modulator based on the three dimensional structure of the druggable region of the polypeptide.

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The present invention also provides a method for identifying a potential modulator of a polypeptide from a database, the method comprising: (a) providing the three-dimensional coordinates for a plurality of the amino acids of a polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); (b) identifying a druggable region of the polypeptide; and (c) selecting from a database at least one potential modulator comprising three dimensional coordinates which indicate that the modulator can bind or interfere with the druggable region. In one embodiment, the modulator is a small molecule.

The present invention also provides a method for preparing a potential modulator of a druggable region contained in a polypeptide, the method comprising: (a) using the atomic coordinates for the backbone atoms of at least about six amino acid residues from a polypeptide of SEQ ID NO: 4, with a root mean square deviation from the backbone atoms of the amino acid residues of not more than 1.5 Å, to generate one or more three-dimensional structures of a molecule comprising a druggable region from the polypeptide; (b) employing one or more of the three dimensional structures of the molecule to design or select a potential modulator of the druggable region; and (c) synthesizing or obtaining the modulator.

The present invention also provides an apparatus for determining whether a compound is a potential modulator of a polypeptide, the apparatus comprising: (a) a memory that comprises: (i) the three dimensional coordinates and identities of at least about fifteen atoms from a druggable region of a polypeptide comprising (1) an amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4: (2) an amino acid sequence having at least about 95% identity with the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; or (3) an amino acid sequence encoded by a polynucleotide that hybridizes under stringent conditions to the complementary strand of a polynucleotide having SEQ ID NO: 1 or SEQ ID NO: 3 and has at least one biological activity of human constitutive androstane receptor (CAR); (ii) executable instructions; and (b) a processor that is capable of executing instructions to: (i) receive three-dimensional structural information for a candidate modulator; (ii) determine if the three-dimensional structure of the candidate modulator is complementary to the three dimensional coordinates of the atoms from the druggable region; and (iii) output the results of the determination.

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The present invention also provides a method for making an inhibitor of constitutive androstane receptor (CAR) activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of constitutive androstane receptor (CAR) activity, the chemical entity having been identified during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or complex, the molecule or complex comprising at least a portion of at least one druggable region from human constitutive androstane receptor (CAR); supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind or to interfere with the molecule or complex at a druggable region, wherein binding to or interfering with the molecule or complex is indicative of potential inhibition of constitutive androstane receptor (CAR) activity.

-23-

The present invention also provides a computer readable storage medium comprising digitally encoded data, wherein the data comprises structural coordinates for a druggable region that is structurally homologous to the structure coordinates as listed in Table 2 or Table 3 for a druggable region of human constitutive androstane receptor (CAR).

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The present invention also provides a computer readable storage medium comprising digitally encoded structural data, wherein the data comprise a majority of the three-dimensional structure coordinates as listed in Table 2 or Table 3. In one embodiment, the computer readable storage medium further comprises the identity of the atoms for the majority of the three-dimensional structure coordinates as listed in Table 2 or Table 3. In another embodiment, the data comprise substantially all of the three-dimensional structure coordinates as listed in Table 2 or Table 3.

The present invention also provides a method for building a model for an activated conformation of a constitutive androstane receptor (CAR), the method comprising: (a) employing coordinates for CAR residues 107 to 332 as shown in Table 2; (b) rotating and translating an X-ray structure of the Vitamin D receptor (VDR), so as to superimpose its core backbone atoms onto corresponding atoms from CAR; (c) combining a superimposed VDR AF2 helix, residues 416-423, with residues 107-332 from CAR from step (a), to provide a starting model for residues 107-332 and 341-348 of CAR in the activated conformation; (d) computationally mutating Val418, Leu419, Val421. Phe422 and Gly423 in the VDR AF2 helix to corresponding amino acids in a CAR AF2 helix, wherein the corresponding amino acids in the CAR AF2 helix are Leu343, Gln344, Ile346, Cys347 and Ser348, respectively; and (e) adjusting the conformations of the mutated amino acid side chains in residues 343, 344, and 346-348 of the AF2 helix of CAR to avoid overlaps, wherein the adjusting is accomplished by one of manual manipulation and conformational search and energy minimization. In one embodiment, the method further comprises modeling a CAR AF2 linker region, residues 333-340, by using a computational loop modeling technique.

-24-

Accordingly, it is an object of the present invention to provide a three-dimensional structure of the ligand-binding domain of CAR in complex with a ligand. The object is achieved in whole or in part by the present invention.

An object of the invention having been stated hereinabove, other objects will be evident as the description proceeds, when taken in connection with the accompanying Drawings and Examples as described hereinbelow.

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Brief Description of the Drawings

Figure 1 is a ribbon diagram depicting the secondary structure of CAR LBD bound with ligand. The ligand is shown as ball and stick. Helices are indicated by H followed by the α helix number, and β -strands are indicated by b followed by the β -strand number. The line at the bottom of the figure indicates the scale, and corresponds to 50 angstroms. N refers to the N-terminus and C refers to the C-terminus.

Figure 2 is a structure-based sequence alignment of the human, mouse, and rat CAR polypeptides with the human PXR polypeptide and the human VDR polypeptide. The residues that make up the α helices are boxed with a light gray line and light gray background. The residues that make up the β sheets are boxed with a darker gray line and darker gray background. The residues within 5Å of the ligand are individually boxed with a thin black square box. Conserved residues are indicated in bold type.

Figure 3 depicts the CAR ligand-binding site. CAR amino acids are shown with light and dark gray lines. A ligand is shown in heavy black lines. The hydrogen bonds between CAR amino acids and the ligand are shown with dotted lines. Particular amino acids that are involved in the ligand binding are indicated using one letter code and amino acid number.

Figure 4 is a stick diagram depicting another view of the ligand-binding site. CAR amino acids are shown with light and dark gray lines. A ligand is shown in heavy black lines. The hydrogen bonds between CAR amino acids and the ligand are shown with dotted lines. Particular amino acids that are involved in the ligand binding are indicated using one letter code and amino acid number.

-25-

Figure 5 depicts the CAR binding pocket. Ligand Compound 1 is shown in Van der Walls ball form. The binding pocket is shown as a dotted surface. The protein backbone is shown in ribbon form. The side chains in the binding pocket are shown in ball and stick form.

Figure 6 depicts another view of the ribbon diagram depicting secondary structure of the three-layer sandwich shaped ligand-binding pocket.

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Figure 7 is a schematic diagram of a general strategy for synthesizing ligands that can bind to the CAR LBD. This scheme is described in Example 6, which outlines the synthesis of an exemplary ligand, Compound 1.

Brief Description of the Sequences in the Sequence Listing

SEQ ID NO: 1 is a DNA sequence encoding a full-length human CAR polypeptide.

15 SEQ ID NO: 2 is an amino acid sequence of a full-length human CAR polypeptide.

SEQ ID NO: 3 is a DNA sequence encoding human CAR residues 103-340, the ligand-binding domain of CAR polypeptide.

SEQ ID NO: 4 is an amino acid sequence of residues 103-340, the ligand-binding domain of CAR polypeptide.

SEQ ID NO: 5 is a His tag amino acid sequence.

SEQ ID NO: 6 is a DNA sequence of a primer used in combination with the primer of SEQ ID NO: 7 to amplify a DNA fragment encoding amino acid residues 103 - 348 of a human CAR polypeptide. In addition to amplifying these coding nucleotides, the primer also includes sequences that will result in the amplified product (a) encoding a His tag as in SEQ ID NO: 5; and (b) having an Ndel endonuclease restriction site (CATATG) just 5' to the His tagencoding residues.

SEQ ID NO: 7 is a DNA sequence of a primer used in combination with the primer of SEQ ID NO: 6 to amplify a DNA fragment encoding residues 103 - 348 of a human CAR polypeptide. The sequence of this primer includes a BamHI endonuclease restriction site (GGATCC) 3' to the human CAR

-26-

polypeptide coding residues. When this primer is used in combination with the primer of SEQ ID NO: 6, the amplified product will have the following arrangement of features: Ndel site – His tag – nucleotides encoding human CAR amino acids 103 to 348 – BamHI site.

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Detailed Description of the Invention

Until disclosure of the present invention presented herein, the ability to obtain crystalline forms of a CAR LBD, particularly in complex with an antagonist ligand, has not been realized. And until disclosure of the present invention presented herein, a detailed three-dimensional crystal structure of an unliganded CAR polypeptide or a CAR polypeptide in complex with a ligand has not been solved.

In addition to providing structural information, crystalline polypeptides provide other advantages. For example, the crystallization process itself further purifies the polypeptide, and satisfies one of the classical criteria for homogeneity. In fact, crystallization frequently provides unparalleled purification quality, removing impurities that are not removed by other purification methods such as HPLC, dialysis, conventional column chromatography, etc. Moreover, crystalline polypeptides are often stable at ambient temperatures and free of protease contamination and degradation associated with solution storage. Crystalline polypeptides can also be useful as pharmaceutical preparations. Finally, crystallization techniques are generally free of problems such as denaturation associated with other stabilization methods (e.g., lyophilization).

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Once crystallization has been accomplished, crystallographic data provides useful structural information that can assist the design of compounds that can serve as agonists or antagonists, as described herein below. In addition, the crystal structure provides information that can be used to map the molecular surface of the ligand-binding domain of CAR. A small non-peptide molecule designed to mimic portions of this surface could serve as a modulator of CAR activity.

-27-

I. <u>Definitions</u>

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Before the present proteins, nucleotide sequences, and methods are described, it is understood that this invention is not limited to the particular methodology, protocols, cell lines, vectors, and reagents described, as these can vary. It is also to be understood that the terminology used herein is for the purpose of describing particular embodiments only, and is not intended to limit the scope of the present invention, the invention being defined by the claims.

Unless defined otherwise, all technical and scientific terms used herein are intended to have their ordinary meanings as understood by one of ordinary skill in the art to which this invention pertains. Although any methods and materials similar or equivalent to those described herein can be used in the practice or testing of the present invention, representative methods, devices, and materials are now described. All publications mentioned herein are incorporated by reference for the purpose of describing the cell lines, vectors, reagents, and methodologies they disclose.

Following long-standing patent law convention, the articles "a" and "an" are used herein to refer to one or to more than one (i.e., to at least one) of the grammatical object of the article. By way of example, "an element" means one element or more than one element.

As used herein, the term "AF2 helix" refers to a short alpha-helix, usually including 5-8 residues, located at the C-terminal end of a LBD sequence, that can usually adopt multiple positions, orientations, and conformations in the structure, and which is involved in binding to coactivators. In the hypothetical activated conformation of CAR, the AF2 helix is expected to include residues 341 to 347. These residues do not adopt an alpha-helical conformation in the structure of CAR bound to Compound 1.

As used herein, the terms "Compound 1" and "Formula (A)" are used interchangeably and refer to 2-(benzhydrylamino)-1-(2-phenylethyl)-1H-benzimidazole-6-carboxamide.

As used herein, the term "AF2 glutamate" refers to a glutamate residue in the AF2 helix that can make hydrogen bond interactions with the exposed

NH groups of the LXXLL-containing peptide from a coactivator if the AF2 helix is in the active position. In CAR, the AF2 glutamate is residue number 345.

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As used herein, the terms "activated", "active conformation", and "activated conformation" of an LBD are used interchangeably and refer to a conformation where the AF2 helix is in the active position, thereby placing the AF2 glutamate residue in a position and orientation that creates a charge Similarly, the terms "active clamp that can recruit coactivator peptides. position of the AF2 helix" and "active conformation of the AF2 helix" are used interchangeably and mean an AF2 helix having a position and/or orientation similar to that of the AF2 helix in the PPARg/SRC-1/rosiglitazone structure of Nolte et al., 1998, allowing the AF2 glutamate residue to make interactions with the exposed NH groups of a coactivator peptide. The position and/or orientation of the AF2 helix in an NR structure can be compared with that of the AF2 helix in another NR structure by rotating and/or translating one structure so as to superimpose the backbone atoms of helices 1 through 10 onto the corresponding atoms of the other structure, where corresponding residues are determined by sequence alignment. If, after superimposition, a majority of the backbone atoms of the core of the AF2 helix lie within 2.0 angstroms of the corresponding atoms from the PAPRg/SRC-1/rosiglitazone structure, then the AF2 helix is defined as being in an active position or active conformation.

Other examples of a nuclear receptor where the AF2 helix is in an "active position" include the X-ray structures of the estrogen receptor α (ER α) bound to estradiol (Brzozowski *et al.*, 1997) and diethylstilbesterol (DES) (Shiau *et al.*, 1998). Examples of a nuclear receptor where the AF2 helix is not in an "active position" are the X-ray structures of the estrogen receptor α (ER α) bound to raloxifene (Brzozowski *et al.*, 1997) and tamoxifen (Shiau *et al.*, 1998). Binding of a coactivator, and AF2-dependent activation of gene transcription, normally requires that the AF2 helix be in the "active position" (Nolte *et al.*, 1998; Shiau *et al.*, 1998). This creates a "charge-clamp" structure that holds the coactivator in its required position (Nolte *et al.*, 1998).

As used herein, the terms "repressed", "inactive conformation", and "repressed conformation" of an LBD are used interchangeably and refer to a conformation where the AF2 helix is not in the active position, and where the AF2 glutamate residue is not in a position that could create the charge clamp that can recruit coactivator peptides.

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As used herein, the term "agonist" refers to an agent that supplements or potentiates the biological activity of a functional CAR gene or protein, or of a polypeptide encoded by a gene that is up- or down-regulated by a CAR polypeptide and/or a polypeptide encoded by a gene that contains a CAR binding site or response element in its promoter region. An agent is also an agonist when the changes in gene expression, considered over many genes, are similar in direction to those induced by other agents that are commonly regarded as agonists. In one embodiment, an agonist of CAR is an androstane.

As used herein, the term "antagonist" refers to an agent that decreases or inhibits the biological activity of a functional gene or protein (for example, a functional CAR gene or protein), or that supplements or potentiates the biological activity of a naturally occurring or engineered non-functional gene or protein (for example, a non-functional CAR gene or protein). Alternatively, an antagonist can decrease or inhibit the biological activity of a functional gene or polypeptide encoded by a gene that is up- or down-regulated by a CAR polypeptide and/or contains a CAR binding site or response element in its promoter region. An antagonist can also supplement or potentiate the biological activity of a naturally occurring or engineered non-functional gene or polypeptide encoded by a gene that is up- or down-regulated by a CAR polypeptide, and/or contains a CAR binding site or response element in its promoter region. An agent is also an antagonist when the changes in gene expression, considered over many genes, are opposite in direction to those induced by other agents that are commonly regarded as agonists.

As used herein, the terms " α -helix" and "alpha-helix" are used interchangeably and refer to a conformation of a polypeptide chain wherein the polypeptide backbone is wound around the long axis of the molecule in a

-30-

left-handed or right-handed direction, and the R groups of the amino acids protrude outward from the helical backbone, wherein the repeating unit of the structure is a single turn of the helix, which extends about 0.56 nm along the long axis.

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As used herein, the terms "amino acid", "amino acid residue", and "residue" are used interchangeably and refer to an amino acid formed upon chemical digestion (hydrolysis) of a peptide or polypeptide at its peptide linkages. Amino acids can also be synthesized individually or as components of a peptide. In one embodiment, the amino acid residues described herein are in the "L" isomeric form. However, residues in the "D" isomeric form can be substituted for any L-amino acid residue, provided that the desired functional property is retained by the polypeptide. In the context of an amino acid, NH2 refers to the free amino group present at the amino terminus of a polypeptide, although some amino acids can have NH₂ groups at other positions in the amino acid. COOH refers to the free carboxy group present at the carboxy terminus of a polypeptide. In keeping with standard polypeptide nomenclature, abbreviations for amino acid residues are presented above. The term "amino acid" is intended to embrace all molecules, whether natural or synthetic, which include both an amino functionality and an acid functionality and capable of being included in a polymer of naturally occurring amino acids. Exemplary amino acids include naturally occurring amino acids; analogs, derivatives and congeners thereof; amino acid analogs having variant side chains; and all stereoisomers of any of the foregoing.

It is noted that amino acid residue sequences represented herein by formulae have a left-to-right orientation in the conventional direction of amino terminus to carboxy terminus. In addition, the terms "amino acid", "amino acid residue", and "residue" are broadly defined to include the amino acids listed in the above table and modified or unusual amino acids. Furthermore, it is noted that a dash at the beginning or end of an amino acid residue sequence indicates a peptide bond to a further sequence of one or more amino acid residues or a covalent bond to an amino-terminal group such as NH₂ or acetyl or to a carboxy-terminal group such as COOH.

As used herein, the terms " β -sheet" and "beta-sheet" are used interchangeably and refer to the conformation of a polypeptide chain stretched into an extended zigzag conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains or from each other.

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The term "binding" refers to an association, which can be a stable association, between two molecules, *i.e.*, between a polypeptide of the invention and a binding partner, due to, for example, electrostatic, hydrophobic, ionic, and/or hydrogen-bond interactions under physiological conditions.

As used herein, the terms "binding pocket of the CAR ligand-binding domain", "CAR ligand-binding pocket" and "CAR binding pocket" are used interchangeably, and refer to the large cavity within the CAR ligand-binding domain where a ligand (e.g. Compound 1) binds. This cavity can be empty, or can contain water molecules or other molecules from the solvent, or can contain ligand atoms. The "main" binding pocket includes the region of space not occupied by atoms of CAR that is approximately encompassed or bounded by residues Phe132, Phe161, Ile164, Asn165, Thr166, Met168, Val169, Ala198, Val199, Cys202, His203, Leu206, Phe217, Tyr224, Thr225, Ile226, Glu227, Asp228, Gly229, Ala230, Phe234, Phe238, Leu239, Leu242, Phe243, His246, Tyr326, Ile330, Leu336, Ser337, Met339, and Met340. The binding pocket also includes small regions near to and contiguous with the "main" binding pocket that not occupied by atoms of CAR.

As used herein the term "biological activity" refers to any biochemical function of a biological molecule. A biological activity includes, but is not limited to, an interaction with another biological molecule (for example, a polypeptide or a nucleic acid, or a combination thereof). As such, a biological activity results in a biochemical effect including, but not limited to the initiation or inhibition of transcription of a gene.

The term "complex" refers to an association between at least two moieties (i.e. chemical or biochemical) that have an affinity for one another.

Examples of complexes include associations between antigen/antibodies. lectin/avidin. target polynucleotide/probe oligonucleotide, antibody/antiantibody. receptor/ligand, enzyme/ligand. polypeptide/ polypeptide, polypeptide/polynucleotide, polypeptide/co-factor, polypeptide/substrate. polypeptide/inhibitor, polypeptide/small molecule, and the like. "Member of a complex" refers to one moiety of the complex, such as an antigen or ligand. "Protein complex" or "polypeptide complex" refers to a complex comprising at least one polypeptide.

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The term "conserved residue" refers to an amino acid that is a member of a group of amino acids having certain common properties. The term "conservative amino acid substitution" refers to the substitution (conceptually or otherwise) of an amino acid from one such group with a different amino acid from the same group. A functional way to define common properties between individual amino acids is to analyze the normalized frequencies of amino acid changes between corresponding proteins of homologous organisms (Schulz & Schirmer, 1979). According to such analyses, groups of amino acids can be defined where amino acids within a group exchange preferentially with each other, and therefore resemble each other most in their impact on the overall protein structure (Schulz & Schirmer, 1979). Representative examples of sets of amino acid groups defined in this manner include: (i) a charged group, consisting of Glu and Asp, Lys, Arg and His, (ii) a positively-charged group, consisting of Lys, Arg and His. (iii) a negativelycharged group, consisting of Glu and Asp, (iv) an aromatic group, consisting of Phe, Tyr and Trp, (v) a nitrogen ring group, consisting of His and Trp, (vi) a large aliphatic nonpolar group, consisting of Val, Leu and Ile, (vii) a slightlypolar group, consisting of Met and Cys, (viii) a small-residue group, consisting of Ser, Thr, Asp, Asn, Gly, Ala, Glu, Gln and Pro, (ix) an aliphatic group consisting of Val, Leu, Ile, Met and Cys, and (x) a small hydroxyl group consisting of Ser and Thr.

As used herein, the term "DNA segment" refers to a DNA molecule that has been isolated free of total genomic DNA of a particular species. In one embodiment, a DNA segment encoding a CAR polypeptide refers to a nucleic

acid comprising SEQ ID NO: 1. In another embodiment, a DNA segment encoding a CAR polypeptide refers to a nucleic acid comprising SEQ ID NO: 3. DNA segments can comprise a portion of a recombinant vector, including, for example, a plasmid, a cosmid, a phage, a virus, and the like.

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As used herein, the term "DNA sequence encoding a CAR polypeptide" refers to one or more coding sequences within a particular individual. Moreover, certain differences in nucleotide sequences can exist between individual organisms, which are called alleles. It is possible that such allelic differences might or might not result in differences in amino acid sequence of the encoded polypeptide yet still encode a protein with the same biological activity. As is well known, genes for a particular polypeptide can exist in single or multiple copies within the genome of an individual. Such duplicate genes can be identical or can have certain modifications, including nucleotide substitutions, additions, or deletions, all of which still code for polypeptides having substantially the same activity.

The term "domain", when used in connection with a polypeptide, refers to a specific region within the polypeptide that comprises a particular structure or mediates a particular function. In the typical case, a domain of a polypeptide of the invention is a fragment of the polypeptide. In certain instances, a domain is a structurally stable domain, as evidenced, for example, by mass spectroscopy, or by the fact that a modulator can bind to a druggable region of the domain. In one embodiment, a domain of a CAR polypeptide is a ligand-binding domain. In another embodiment, a domain of a CAR polypeptide is a DNA-binding domain.

The term "druggable region", when used in reference to a polypeptide, nucleic acid, complex and the like, refers to a region of the molecule that is a target or is a likely target for binding a modulator. For a polypeptide, a druggable region generally refers to a region wherein several amino acids of a polypeptide would be capable of interacting with a modulator or other molecule. For a polypeptide or complex thereof, exemplary druggable regions including binding pockets and sites, enzymatic active sites, interfaces between domains of a polypeptide or complex, surface grooves or contours or

surfaces of a polypeptide or complex which are capable of participating in interactions with another molecule. In certain instances, the interacting molecule is another polypeptide, which can be naturally occurring. In other instances, the druggable region is on the surface of the molecule. In one embodiment, a druggable region of a CAR polypeptide comprises the binding site defined by amino acid residues 103-340. In another embodiment, a druggable region of a CAR polypeptide comprises amino acid residues and surfaces of the CAR polypeptide that interact with a RXR polypeptide during CAR-RXR heterodimer formation. In another embodiment, a druggable region of a CAR polypeptide comprises the AF2 helix. In another embodiment, a druggable region of a CAR polypeptide comprises Glu345. In still another embodiment, a druggable region of a CAR polypeptide comprises a DNA-binding domain.

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Druggable regions can be described and characterized in a number of ways. For example, a druggable region can be characterized by some or all of the amino acids that make up the region, or the backbone atoms thereof, or the side chain atoms thereof (optionally with or without the $C\alpha$ atoms). Alternatively, in certain instances, the volume of a druggable region corresponds to that of a carbon based molecule of at least about 200 atomic mass units (amu) and often up to about 800 amu. In other instances, it will be appreciated that the volume of such region can correspond to a molecule of at least about 600 amu and often up to about 1600 amu or more.

Alternatively, a druggable region can be characterized by comparison to other regions on the same or other molecules. For example, the term "affinity region" refers to a druggable region on a molecule (such as a polypeptide of the invention) that is present in several other molecules, in so much as the structures of the same affinity regions are sufficiently the same so that they are expected to bind the same or related structural analogs. An example of an affinity region is an ATP-binding site of a protein kinase that is found in several protein kinases (whether or not of the same origin). Another example of an affinity region is a DNA-binding domain: for example, the DNA-binding domain of a CAR polypeptide.

In contrast to an affinity region, the term "selectivity region" refers to a druggable region of a molecule that can not be found on other molecules, in so much as the structures of different selectivity regions are sufficiently different so that they are not expected to bind the same or related structural analogs. An exemplary selectivity region is a catalytic domain of a protein kinase that exhibits specificity for one substrate. In certain instances, a single modulator can bind to the same affinity region across a number of proteins that have a substantially similar biological function, whereas the same modulator can bind to only one selectivity region of one of those proteins.

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Continuing with examples of different druggable regions, the term "undesired region" refers to a druggable region of a molecule that upon interacting with another molecule results in an undesirable affect. For example, a binding site that oxidizes the interacting molecule and thereby results in increased toxicity for the oxidized molecule can be deemed an "undesired region". Other examples of potential undesired regions include regions that upon interaction with a drug decrease the membrane permeability of the drug, increase the excretion of the drug, or increase the blood brain transport of the drug. It can be the case that, in certain circumstances, an undesired region will no longer be deemed an undesired region because the affect of the region will be favorable, *i.e.*, a drug intended to treat a brain condition would benefit from interacting with a region that resulted in increased blood brain transport, whereas the same region could be deemed undesirable for drugs that were not intended to be delivered to the brain.

When used in reference to a druggable region, the "selectivity" or "specificity' of a molecule such as a modulator to a druggable region can be used to describe the binding between the molecule and a druggable region. For example, the selectivity of a modulator with respect to a druggable region can be expressed by comparison to another modulator, using the respective values of K_d (*i.e.*, the dissociation constants for each modulator-druggable region complex) or, in cases where a biological effect is observed below the K_d , the ratio of the respective EC_{50} 's (*i.e.*, the concentrations that produce

-36-

50% of the maximum response for the modulator interacting with each druggable region).

As used herein, the term "expression" generally refers to the cellular processes by which a biologically active polypeptide is produced. As such, the term "expression" generally includes those cellular processes that begin with transcription and end with the production of a functional polypeptide. As used herein, "expression" is also intended to refer to cellular processes by which a polypeptide is produced that would otherwise be functional except for the presence of mutations in the nucleotide sequence encoding it. Consistent with this usage, "expression" includes, but is not limited to, such processes as transcription, translation, post-translational modification, and transport of a polypeptide.

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A "fusion protein" or "fusion polypeptide" refers to a chimeric protein as that term is known in the art and can be constructed using methods known in the art. In many examples of fusion proteins, there are two different polypeptide sequences, and in certain cases, there can be more. sequences can be linked in frame. A fusion protein can include a domain that is found (albeit in a different protein) in an organism that also expresses the first protein, or it can be an "interspecies", "intergenic", etc. fusion expressed by different kinds of organisms. In various embodiments, the fusion polypeptide can comprise one or more amino acid sequences linked to a first polypeptide. In the case where more than one amino acid sequence is fused to a first polypeptide, the fusion sequences can be multiple copies of the same sequence, or alternatively, can be different amino acid sequences. The fusion polypeptides can be fused to the N-terminus, the C-terminus, or the Nand C-terminus of the first polypeptide. Exemplary fusion proteins include polypeptides comprising a glutathione S-transferase tag (GST-tag), histidine tag (His-tag), an immunoglobulin domain, or an immunoglobulin-binding domain.

As used herein, the term "gene" is used for simplicity to refer to a nucleotide sequence that encodes a protein, a polypeptide, or a peptide. As such, the term "gene" refers to a nucleic acid comprising an open reading

-37-

frame encoding a polypeptide having exon sequences and, optionally, intron sequences. The term "intron" refers to a DNA sequence present in a given gene that is not translated into protein and is generally found between exons. As will be understood by those of skill in the art, this functional term includes both genomic sequences and cDNA sequences. Representative embodiments of such sequences are disclosed herein.

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The term "having substantially similar biological activity", when used in reference to two polypeptides, refers to a biological activity of a first polypeptide which is substantially similar to at least one of the biological activities of a second polypeptide. A substantially similar biological activity means that the polypeptides carry out a similar function, i.e., a similar enzymatic reaction or a similar physiological process, etc. For example, two homologous proteins can have a substantially similar biological activity if they are involved in a similar enzymatic reaction, i.e., they are both kinases which catalyze phosphorylation of a substrate polypeptide, however, they can phosphorylate different regions on the same protein substrate or different substrate proteins altogether. Alternatively, two homologous proteins can also have a substantially similar biological activity if they are both involved in a similar physiological process, i.e., regulation of transcription. For example, two proteins can be transcription factors, however, they can bind to different DNA sequences or bind to different polypeptide interactors. Substantially similar biological activities can also be associated with proteins carrying out a similar structural role, for example, two membrane proteins.

As used herein, the term "interact" refers to detectable interactions between molecules, such as can be detected using, for example, a yeast two-hybrid assay. The term "interact" is also meant to include "binding" interactions between molecules. Interactions include, but are not limited to protein-protein, protein-nucleic acid, and protein-small molecule interactions. These interactions can be in the form of covalent or non-covalent interactions including, but not limited to ionic, hydrogen bonding, and van der Waals interactions.

As used herein, the term "isolated" refers to a nucleic acid substantially free of other nucleic acids, proteins, lipids, carbohydrates, or other materials with which it can be associated, such association being either in cellular material or in a synthesis medium. The term can also be applied to polypeptides, in which case the polypeptide is substantially free of nucleic acids, carbohydrates, lipids, and other undesired polypeptides. The term "isolated polypeptide" refers to a polypeptide, in certain embodiments prepared from recombinant DNA or RNA, or of synthetic origin, or some combination thereof, which (1) is not associated with proteins that it is normally found with in nature, (2) is isolated from the cell in which it normally occurs, (3) is isolated free of other proteins from the same cellular source, (4) is expressed by a cell from a different species, or (5) does not occur in nature.

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The term "isolated nucleic acid" refers to a polynucleotide of genomic, cDNA, or synthetic origin or some combination there of, which (1) is not associated with the cell in which the "isolated nucleic acid" is found in nature, or (2) is operably linked to a polynucleotide to which it is not linked in nature.

The terms "label" or "labeled" refer to incorporation or attachment, optionally covalently or non-covalently, of a detectable marker into a molecule, such as a polypeptide. Various methods of labeling polypeptides are known in the art and can be used. Examples of labels for polypeptides include, but are not limited to the following: radioisotopes, fluorescent labels, heavy atoms, enzymatic labels or reporter genes, chemiluminescent groups, biotinyl groups, predetermined polypeptide epitopes recognized by a secondary reporter (*i.e.*, leucine zipper pair sequences, binding sites for secondary antibodies, metal binding domains, epitope tags). Examples and use of such labels are well known by the skilled artisan. In some embodiments, spacer arms of various lengths can be attached to labels to reduce potential steric hindrance.

The term "mammal" is known in the art, and exemplary mammals include humans, primates, bovines, porcines, canines, felines, and rodents (*i.e.*, mice and rats).

The term "modulation", when used in reference to a functional property or biological activity or process (i.e., enzyme activity or receptor binding), refers to the capacity to up regulate (i.e., activate or stimulate), down regulate (i.e., inhibit or suppress), or otherwise change a quality of such property, activity, or process. In certain instances, such regulation can be contingent on the occurrence of a specific event, such as activation of a signal transduction pathway, and/or can be manifest only in particular cell types.

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The term "modulator" refers to a polypeptide, nucleic acid, macromolecule, complex, molecule, small molecule, compound, species, or the like (naturally-occurring or non-naturally-occurring), or an extract made from biological materials such as bacteria, plants, fungi, or animal cells or tissues, that can be capable of causing modulation. Modulators can be evaluated for potential activity as inhibitors or activators (directly or indirectly) of a functional property, biological activity or process, or combination thereof, (i.e., agonist, partial antagonist, partial agonist, inverse agonist, antagonist, anti-microbial agents, inhibitors of microbial infection or proliferation, and the like) by inclusion in assays. In such assays, many modulators can be screened at one time. The activity of a modulator can be known, unknown, or partially known.

As used herein, the term "molecular replacement" refers to a method that involves generating a preliminary model of the wild-type CAR ligand-binding domain, or a CAR mutant crystal the structure for which coordinates are unknown, by orienting and positioning a molecule the structure for which coordinates are known (e.g., the vitamin D receptor; VDR) within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure the coordinates for which are unknown. This, in turn, can be subjected to any of the several forms of refinement known in the art to provide a final, accurate structure of the unknown crystal (see e.g. Lattman, 1985; Rossmann, 1972). Using the structure coordinates of the ligand-binding domain of CAR provided by this invention, molecular

-40-

replacement can be used to determine the structure coordinates of a crystal of a mutant or of a homologue of the CAR ligand-binding domain, or of a different crystal form of the CAR ligand-binding domain.

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The term "motif" refers to an amino acid sequence that is commonly found in a protein of a particular structure or function. Typically, a consensus sequence is defined to represent a particular motif. The consensus sequence need not be strictly defined and can contain positions of variability, degeneracy, variability of length, etc. The consensus sequence can be used to search a database to identify other proteins that can have a similar structure or function due to the presence of the motif in its amino acid For example, on-line databases can be searched with a sequence. consensus sequence in order to identify other proteins containing a particular motif. Various search algorithms and/or programs can be used, including FASTA, BLAST, or ENTREZ. FASTA and BLAST are available as a part of the GCG sequence analysis package (Accelrys, Inc., San Diego, California, United States of America). ENTREZ is available through the National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, Bethesda, Maryland, United States of America.

As used herein, the term "mutation" carries its traditional connotation and refers to a change, inherited, naturally occurring, or introduced, in a nucleic acid or polypeptide sequence, and is used in its sense as generally known to those of skill in the art.

The term "naturally occurring", as applied to an object, refers to the fact that an object can be found in nature. For example, a polypeptide or polynucleotide sequence that is present in an organism (including bacteria) that can be isolated from a source in nature and which has not been intentionally modified by man in the laboratory is naturally occurring.

The term "nucleic acid" refers to a polymeric form of nucleotides, either ribonucleotides or deoxynucleotides or a modified form of either type of nucleotide. The terms should also be understood to include, as equivalents, analogs of either RNA or DNA made from nucleotide analogs, and, as

applicable to the embodiment being described, single-stranded (such as sense or antisense) and double-stranded polynucleotides.

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The term "nucleic acid of the invention" refers to a nucleic acid encoding a polypeptide of the invention, i.e., a nucleic acid comprising a sequence consisting of, or consisting essentially of, the polynucleotide sequence set forth in SEQ ID NO: 1 or SEQ ID NO: 3. A nucleic acid of the invention can comprise all, or a portion of: the nucleotide sequence of SEQ ID NO: 1 or SEQ ID NO: 3; a nucleotide sequence at least 60%, 70%, 80%, 90%, 95%, 96%, 97%, 98% or 99% identical to SEQ ID NO: 1 or SEQ ID NO: 3; a nucleotide sequence that hybridizes under stringent conditions to SEQ ID NO: 1 or SEQ ID NO: 3; nucleotide sequences encoding polypeptides that are functionally equivalent to polypeptides of the invention; nucleotide sequences encoding polypeptides at least about 60%, 70%, 80%, 85%, 90%, 95%, 98%, 99% homologous or identical with an amino acid sequence of SEQ ID NO: 2 or SEQ ID NO: 4; nucleotide sequences encoding polypeptides having an activity of a polypeptide of the invention and having at least about 60%, 70%, 80%. 85%, 90%, 95%, 98%, 99% or more homology or identity with SEQ ID NO: 2 or SEQ ID NO: 4; nucleotide sequences that differ by 1 to about 2, 3, 5, 7, 10, 15, 20, 30, 50, 75 or more nucleotide substitutions, additions or deletions, such as allelic variants, of SEQ ID NO: 1 and SEQ ID NO: 3: nucleic acids derived from and evolutionarily related to SEQ ID NO: 1 or SEQ ID NO: 3; and complements of and nucleotide sequences resulting from the degeneracy of the genetic code, for all of the foregoing and other nucleic acids of the invention. Nucleic acids of the invention also include homologs, i.e., orthologs and paralogs, of SEQ ID NO: 1 or SEQ ID NO: 3 and also variants of SEQ ID NO: 1 or SEQ ID NO: 3 which have been codon optimized for expression in a particular organism (i.e., host cell).

The term "operably linked", when describing the relationship between two nucleic acid regions, refers to a juxtaposition wherein the regions are in a relationship permitting them to function in their intended manner. For example, a control sequence "operably linked" to a coding sequence is ligated in such a way that expression of the coding sequence is achieved under

-42-

conditions compatible with the control sequences, such as when the appropriate molecules (i.e., inducers and polymerases) are bound to the control or regulatory sequence(s).

As used herein, "orthorhombic unit cell" refers to a unit cell wherein a \neq b \neq c, and $\alpha = \beta = \gamma = 90^{\circ}$. The vectors a, b, and c describe the unit cell edges and the angles α , β , and γ describe the unit cell angles.

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As used herein, the term "CAR" refers to any polypeptide with an amino acid sequence that can be aligned with at least one of human, mouse, or rat CAR, such that at least 50% of the amino acids are identical to the corresponding amino acid in the human, mouse, or rat CAR. The term "CAR" also encompasses nucleic acids for which the corresponding translated protein sequence can be considered to be a CAR. The term "CAR" includes vertebrate homologs of CAR family members including, but not limited to mammalian and avian homologs. Representative mammalian homologs of CAR family members include, but are not limited to murine and human homologs.

As used herein, the terms "CAR gene" and "recombinant CAR gene" are used interchangeably and refer to a nucleic acid molecule comprising an open reading frame encoding a CAR polypeptide, including both exon and (optionally) intron sequences.

As used herein, the terms "CAR gene product", "CAR protein", "CAR polypeptide", and "CAR peptide" are used interchangeably and refer to peptides having amino acid sequences which are substantially identical to native CAR amino acid sequences from the organism of interest and which are biologically active in that they comprise all or a part of the amino acid sequence of a CAR polypeptide, or cross-react with antibodies raised against a CAR polypeptide, or retain all or some of the biological activity (e.g., DNA or ligand-binding ability and/or dimerization ability) of the native amino acid sequence or protein. Such biological activity can include immunogenicity.

As used herein, the terms "CAR gene product", "CAR protein", "CAR polypeptide", and "CAR peptide" are used interchangeably and refer to a subtype of the CAR family. In one embodiment, a CAR gene product is CAR.

-43-

In another embodiment, a CAR gene product comprises the amino acid sequence of SEQ ID NO: 2.

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As used herein, the terms "CAR gene product", "CAR protein". "CAR polypeptide", and "CAR peptide" also include analogs of a CAR polypeptide. By "analog" is intended that a DNA or peptide sequence can contain alterations relative to the sequences disclosed herein, yet retain all or some of the biological activity of those sequences. Analogs can be derived from genomic nucleotide sequences as are disclosed herein or those from other organisms, or can be created synthetically. Those skilled in the art will appreciate that other analogs, as yet undisclosed or undiscovered, can be used to design and/or construct CAR analogs. There is no need for a "CAR gene product", "CAR protein", "CAR polypeptide", or "CAR peptide" to comprise all or substantially all of the amino acid sequence of a CAR polypeptide gene product. Shorter or longer sequences are anticipated to be of use in the invention; shorter sequences are herein referred to as Thus, the terms "CAR gene product", "CAR protein", "CAR "seaments". polypeptide", and "CAR peptide" also include fusion or recombinant CAR polypeptides and proteins comprising sequences of the present invention. Methods of preparing such proteins are disclosed herein and are known in the art.

The term "phenotype" refers to the entire physical, biochemical, and physiological makeup of a cell, *i.e.*, having any one trait or any group of traits.

As used herein, the term "polypeptide" refers to any polymer comprising any of the 20 protein amino acids, regardless of its size. Although "protein" is often used in reference to relatively large polypeptides and "peptide" is often used in reference to small polypeptides, usage of these terms in the art overlaps and varies. The term "polypeptide" as used herein refers to peptides, polypeptides, and proteins, unless otherwise noted. As used herein, the terms "protein", "polypeptide" and "peptide" are used interchangeably herein when referring to a gene product. The term "polypeptide", and the terms "protein" and "peptide" which are used interchangeably herein, refers to a polymer of amino acids. Exemplary

-44-

polypeptides include gene products, naturally occurring proteins, homologs, orthologs, paralogs, fragments, as well as other equivalents, variants, and analogs of the foregoing.

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The terms "polypeptide fragment" or "fragment", when used to refer to a reference polypeptide, refers to a polypeptide in which amino acid residues are deleted as compared to the reference polypeptide itself, but where the remaining amino acid sequence is usually identical to the corresponding positions in the reference polypeptide. Such deletions can occur at the amino-terminus or carboxy-terminus of the reference polypeptide, or alternatively both. Fragments typically are at least 5, 6, 8 or 10 amino acids long, at least 14 amino acids long, at least 20, 30, 40 or 50 amino acids long, at least 75 amino acids long, or at least 100, 150, 200, 300, 500 or more amino acids long. A fragment can retain one or more of the biological activities of the reference polypeptide. In certain embodiments, a fragment can comprise a druggable region, and optionally additional amino acids on one or both sides of the druggable region, which additional amino acids can number from 5, 10, 15, 20, 30, 40, 50, or up to 100 or more residues. Further, fragments can include a sub-fragment of a specific region, which subfragment retains a function of the region from which it is derived. In one embodiment, a fragment can have immunogenic properties.

The term "polypeptide of the invention" refers to a polypeptide comprising the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4, or an equivalent or fragment thereof: *i.e.*, a polypeptide comprising a sequence consisting of, or consisting essentially of, the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4. Polypeptides of the invention include polypeptides comprising all or a portion of the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4; the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4 with 1 to about 2, 3, 5, 7, 10, 15, 20, 30, 50, 75 or more conservative amino acid substitutions; an amino acid sequence that is at least 60%, 70%, 80%, 90%, 95%, 96%, 97%, 98%, or 99% identical to SEQ ID NO: 2 or SEQ ID NO: 4; and functional fragments

-45-

thereof. Polypeptides of the invention also include homologs, i.e., orthologs and paralogs, of SEQ ID NO: 2 or SEQ ID NO: 4.

As used herein, the term "primer" refers to a nucleic acid comprising in one embodiment 2 or more deoxyribonucleotides or ribonucleotides, in another embodiment more than 3, in another embodiment more than 8, and in yet another embodiment at least about 20 nucleotides of an exonic or intronic region. In one embodiment, an oligonucleotide is between 10 and 30 bases in length.

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The term "purified" refers to an object species that is the predominant species present (i.e., on a molar basis it is more abundant than any other individual species in the composition). A "purified fraction" is a composition wherein the object species comprises at least about 50 percent (on a molar basis) of all species present. In making the determination of the purity of a species in solution or dispersion, the solvent or matrix in which the species is dissolved or dispersed is usually not included in such determination; instead, only the species (including the one of interest) dissolved or dispersed are taken into account. Generally, a purified composition will have one species that comprises more than about 80 percent of all species present in the composition, more than about 85%, 90%, 95%, 99% or more of all species The object species can be purified to essential homogeneity present. (contaminant species cannot be detected in the composition by conventional detection methods) wherein the composition consists essentially of a single species. A skilled artisan can purify a polypeptide of the invention using standard techniques for protein purification in light of the teachings herein. Purity of a polypeptide can be determined by a number of methods known to those of skill in the art, including for example, amino-terminal amino acid sequence analysis, gel electrophoresis, mass-spectrometry analysis and the methods described herein.

The terms "recombinant protein" and "recombinant polypeptide" refer to a polypeptide that is produced by recombinant DNA techniques. An example of such techniques includes when DNA encoding a polypeptide is inserted

into a suitable expression vector that is in turn used to transform a host cell to produce the polypeptide encoded by the DNA.

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A "reference sequence" is a defined sequence used as a basis for a sequence comparison. A reference sequence can be a subset of a larger sequence, for example, as a segment of a full-length protein given in a sequence listing such as SEQ ID NO: 2 or SEQ ID NO: 4, or can comprise a complete protein sequence. Generally, a reference sequence is at least 200, 300 or 400 nucleotides in length, frequently at least 600 nucleotides in length, and often at least 800 nucleotides in length (or the protein equivalent if it is shorter or longer in length). Because two proteins can each (1) comprise a sequence (i.e., a portion of the complete protein sequence) that is similar between the two proteins, and (2) can further comprise a sequence that is divergent between the two proteins, sequence comparisons between two (or more) proteins are typically performed by comparing sequences of the two proteins over a "comparison window" to identify and compare local regions of sequence similarity.

A "comparison window," as used herein, refers to a conceptual segment of at least 20 contiguous amino acid positions wherein a protein sequence can be compared to a reference sequence of at least 20 contiguous amino acids and wherein the portion of the protein sequence in the comparison window can comprise additions or deletions (i.e., gaps) of 20 percent or less as compared to the reference sequence (which does not comprise additions or deletions) for optimal alignment of the two sequences. Optimal alignment of sequences for aligning a comparison window can be conducted by the local homology algorithm of Smith & Waterman, 1981, by the homology alignment algorithm of Needleman & Wunsch, 1970, by the search for similarity method of Pearson & Lipman, 1988, by computerized implementations of these algorithms (GAP, BESTFIT, FASTA, and TFASTA in the Wisconsin Genetics Software Package, available from Accelrys, Inc., San Diego, California, United States of America), or by inspection, and the best alignment (i.e., resulting in the highest percentage of homology over the comparison window) generated by the various methods can be identified.

-47-

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The term "regulatory sequence" is a generic term used throughout the specification to refer to polynucleotide sequences, such as initiation signals, enhancers, regulators and promoters, that are necessary or desirable to affect the expression of coding and non-coding sequences to which they are operably linked. Exemplary regulatory sequences are described in Goeddel. 1990, and include, for example, the early and late promoters of SV40, adenovirus or cytomegalovirus immediate early promoter, the lac system, the trp system, the TAC or TRC system, T7 promoter whose expression is directed by T7 RNA polymerase, the major operator and promoter regions of phage lambda, the control regions for fd coat protein, the promoter for 3phosphoglycerate kinase or other glycolytic enzymes, the promoters of acid phosphatase, i.e., Pho5, the promoters of the yeast α-mating factors, the polyhedron promoter of the baculovirus system and other sequences known to control the expression of genes of prokaryotic or eukaryotic cells or their viruses, and various combinations thereof. The nature and use of such control sequences can differ depending upon the host organism. prokaryotes, such regulatory sequences generally include promoter, ribosomal binding site, and transcription termination sequences. The term "regulatory sequence" is intended to include, at a minimum, components whose presence can influence expression, and can also include additional components whose presence is advantageous, for example, leader sequences and fusion partner sequences. In certain embodiments, transcription of a polynucleotide sequence is under the control of a promoter sequence (or other regulatory sequence) that controls the expression of the polynucleotide in a cell-type in which expression is intended. It will also be understood that the polynucleotide can be under the control of regulatory sequences that are the same or different from those sequences which control expression of the naturally occurring form of the polynucleotide.

The term "reporter gene" refers to a nucleic acid comprising a nucleotide sequence encoding a protein that is readily detectable either by its presence or activity, including, but not limited to, luciferase, fluorescent protein (i.e., green fluorescent protein), chloramphenicol acetyl transferase, β -

-48-

galactosidase, secreted placental alkaline phosphatase, β -lactamase, human growth hormone, and other secreted enzyme reporters. Generally, a reporter gene encodes a polypeptide not otherwise produced by the host cell, which is detectable by analysis of the cell(s), *i.e.*, by the direct fluorometric, radioisotopic or spectrophotometric analysis of the cell(s) and preferably without the need to kill the cells for signal analysis. In certain instances, a reporter gene encodes an enzyme, which produces a change in fluorometric properties of the host cell, which is detectable by qualitative, quantitative, or semiquantitative function or transcriptional activation. Exemplary enzymes include esterases, β -lactamase, phosphatases, peroxidases, proteases (tissue plasminogen activator or urokinase) and other enzymes whose function can be detected by appropriate chromogenic or fluorogenic substrates known to those skilled in the art or developed in the future.

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The term "sequence homology" refers to the proportion of base matches between two nucleic acid sequences or the proportion of amino acid matches between two amino acid sequences. When sequence homology is expressed as a percentage, i.e., 50%, the percentage denotes the proportion of matches over the length of sequence from a desired sequence (i.e., SEQ. ID NO: 1) that is compared to some other sequence. Gaps (in either of the two sequences) are permitted to maximize matching; gap lengths of 15 bases or less are usually used, 6 bases or less are used more frequently, with 2 bases or less used even more frequently. The term "sequence identity" means that sequences are identical (i.e., on a nucleotide-by-nucleotide basis for nucleic acids or amino acid-by-amino acid basis for polypeptides) over a The term "percentage of sequence identity" is window of comparison. calculated by comparing two optimally aligned sequences over the comparison window, determining the number of positions at which the identical amino acids occurs in both sequences to yield the number of matched positions, dividing the number of matched positions by the total number of positions in the comparison window, and multiplying the result by 100 to yield the percentage of sequence identity. Methods to calculate

-49-

sequence identity are known to those of skill in the art and described in further detail herein.

As used herein, the term "sequencing" refers to determining the ordered linear sequence of nucleotides or amino acids of a DNA, RNA, or protein target sample, using conventional manual or automated laboratory techniques.

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The term "small molecule" refers to a compound, which has a molecular weight of less than about 5 kilodalton (kD), less than about 2.5 kD, less than about 1.5 kD, or less than about 0.9 kD. Small molecules can be, for example, nucleic acids, peptides, polypeptides, peptide nucleic acids, peptidomimetics, carbohydrates, lipids, or other organic (carbon containing) or inorganic molecules. The term "small organic molecule" refers to a small molecule that is often identified as being an organic or medicinal compound, and does not include molecules that are exclusively nucleic acids, peptides, or polypeptides.

The term "soluble" as used herein with reference to a polypeptide of the invention or other protein means that upon expression in cell culture, at least some portion of the polypeptide or protein expressed remains in the cytoplasmic fraction of the cell and does not fractionate with the cellular debris upon lysis and centrifugation of the lysate. Solubility of a polypeptide can be increased by a variety of art recognized methods, including fusion to a heterologous amino acid sequence, deletion of amino acid residues, amino acid substitution (i.e., enriching the sequence with amino acid residues having hydrophilic side chains), and chemical modification (i.e., addition of hydrophilic groups). The solubility of polypeptides can be measured using a variety of art recognized techniques, including dynamic light scattering to determine aggregation state, UV absorption, centrifugation to separate aggregated from non-aggregated material, and SDS gel electrophoresis (i.e., the amount of protein in the soluble fraction is compared to the amount of protein in the soluble and insoluble fractions combined). When expressed in a host cell, the polypeptides of the invention can be at least about 1%, 2%, 5%, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90% or more soluble, i.e.,

at least about 1%, 2%, 5%, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90% or more of the total amount of protein expressed in the cell is found in the cytoplasmic fraction. In certain embodiments, a one liter culture of cells expressing a polypeptide of the invention will produce at least about 0.1, 0.2, 0.5, 1, 2, 5, 10, 20, 30, 40, 50 milligrams or more of soluble protein. In an exemplary embodiment, a polypeptide of the invention is at least about 10% soluble and will produce at least about 1 milligram of protein from a one liter cell culture.

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As used herein, the term "space group" refers to the arrangement of symmetry elements of a crystal.

The term "specifically hybridizes" refers to detectable and specific nucleic acid binding. Polynucleotides, oligonucleotides, and nucleic acids of the invention selectively hybridize to nucleic acid strands under hybridization and wash conditions that minimize appreciable amounts of detectable binding to nonspecific nucleic acids. Stringent conditions can be used to achieve selective hybridization conditions as known in the art and discussed herein. Generally, the nucleic acid sequence homology between the polynucleotides, oligonucleotides, and nucleic acids of the invention and a nucleic acid sequence of interest will be at least 30%, 40%, 50%, 60%, 70%, 80%, 85%, 90%, 95%, 98%, 99%, or more. In certain instances, hybridization and washing conditions are performed under stringent conditions according to conventional hybridization procedures and as described further herein.

As used herein, the terms "structure coordinates", "atomic coordinates", and "structural coordinates" are used interchangeably and refer to coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Those of skill in the art understand that a set of coordinates determined by X-ray crystallography is not without experimental error. In general, the

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error in the coordinates tends to be reduced as the resolution is increased, since more experimental diffraction data is available for the model fitting and refinement. Thus, for example, more diffraction data can be collected from a crystal that diffracts to a resolution of 2.0 angstroms than from a crystal that diffracts to a lower resolution, such as 2.5 or 3.0 angstroms. Consequently, the refined structural coordinates will usually be more accurate when fitted and refined using data from a crystal that diffracts to higher resolution. The design of ligands for a CAR polypeptide depends on the accuracy of the structural coordinates. If the coordinates are not sufficiently accurate, then the design process will be ineffective. In most cases, it is very difficult or impossible to collect sufficient diffraction data to define atomic coordinates precisely when the crystals diffract to a resolution of 3.0 angstroms or poorer. Thus, in most cases, it is difficult to use X-ray structures in structure-based ligand design when the X-ray structures are based on crystals that diffract to a resolution of only 3.0 angstroms or poorer. However, common experience has shown that crystals diffracting to 2.0-2.5 angstroms or better can yield Xray structures with sufficient accuracy to greatly facilitate structure-based drug design. Further improvement in the resolution can further facilitate structurebased design, but the coordinates obtained at 2.0-2.5 angstroms resolution are generally considered adequate for most purposes.

Also, those of skill in the art will understand that nuclear receptors can adopt different conformations when different ligands are bound, or in the absence of any ligand. In particular, in most nuclear receptors, the AF2 helix can adopt different conformations when agonists and antagonists (or inverse agonists) are bound. More subtle conformational changes occur in other parts of the LBD when the AF2 helix is shifted. Generally, structure-based design of ligands that modulate CAR activity requires an understanding of the "activated" conformation that occurs when agonists are bound (or in the absence of ligand), as well as the "repressed" conformation that occurs when antagonists (or inverse agonists) are bound. The crystal structure of CAR bound to Compound 1 provides the "repressed" structure of CAR. In one embodiment, the "activated" conformation of CAR can be modeled

approximately by using the "repressed" CAR structure as a starting structure, and then adjusting the conformation of the residues at the C-terminal end of the structure, residues 332-348, to form an AF2 helix with conformation, position, and orientation similar to that observed in the "activated" conformations of other nuclear receptors. It should be noted that the X-ray structure of CAR bound to Compound 1, which is an inverse agonist, revealed a completely novel, unexpected conformation for the residues that normally comprise the AF2 helix and the AF2 linking segment. No conventional modeling procedure could have predicted this novel "repressed" structure from an X-ray structure of the "activated" conformation of CAR.

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The terms "stringent conditions" or "stringent hybridization conditions" refer to conditions that promote specific hybridization between two complementary polynucleotide strands so as to form a duplex. Stringent conditions can be selected to be about 5°C lower than the thermal melting point (Tm) for a given polynucleotide duplex at a defined ionic strength and pH. The length of the complementary polynucleotide strands and their GC content will determine the Tm of the duplex, and thus the hybridization conditions necessary for obtaining a desired specificity of hybridization. The Tm is the temperature (under defined ionic strength and pH) at which 50% of a polynucleotide sequence hybridizes to a perfectly matched complementary strand. In certain cases it can be desirable to increase the stringency of the hybridization conditions to be about equal to the Tm for a particular duplex.

A variety of techniques for estimating the Tm are available. Typically, G-C base pairs in a duplex are estimated to contribute about 3°C to the Tm, while A-T base pairs are estimated to contribute about 2°C, up to a theoretical maximum of about 80-100°C. However, more sophisticated models of Tm are available in which G-C stacking interactions, solvent effects, the desired assay temperature and the like are taken into account. For example, probes can be designed to have a dissociation temperature (Td) of approximately 60°C, using the formula: Td = ((((((3 x #GC) + (2 x #AT)) x 37) - 562)/#bp) - 5; where #GC, #AT, and #bp are the number of guanine-cytosine base pairs, the

-53-

number of adenine-thymine base pairs, and the number of total base pairs, respectively, involved in the formation of the duplex.

Hybridization can be carried out in 5x SSC, 4x SSC, 3x SSC, 2x SSC, 1x SSC or 0.2x SSC for at least about 1 hour, 2 hours, 5 hours, 12 hours, or 24 hours. The temperature of the hybridization can be increased to adjust the stringency of the reaction, for example, from about 25°C (room temperature), to about 45°C, 50°C, 55°C, 60°C, or 65°C. The hybridization reaction can also include another agent affecting the stringency; for example, hybridization conducted in the presence of 50% formamide increases the stringency of hybridization at a defined temperature.

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The hybridization reaction can be followed by a single wash step, or two or more wash steps, which can be at the same or a different salinity and temperature. For example, the temperature of the wash can be increased to adjust the stringency from about 25°C (room temperature), to about 45°C, 50°C, 55°C, 60°C, 65°C, or higher. The wash step can be conducted in the presence of a detergent, *i.e.*, 0.1 or 0.2% SDS. For example, hybridization can be followed by two wash steps at 65°C each for about 20 minutes in 2x SSC, 0.1% SDS, and optionally two additional wash steps at 65°C each for about 20 minutes in 0.2x SSC, 0.1% SDS.

Exemplary stringent hybridization conditions include overnight hybridization at 65°C in a solution comprising, or consisting of, 50% formamide, 10x Denhardt's Solution (0.2% Ficoll, 0.2% Polyvinylpyrrolidone, 0.2% bovine serum albumin) and 200 µg/ml of denatured carrier DNA, *i.e.*, sheared salmon sperm DNA, followed by two wash steps at 65°C each for about 20 minutes in 2x SSC, 0.1% SDS, and two wash steps at 65°C each for about 20 minutes in 0.2x SSC, 0.1% SDS.

Hybridization can include hybridizing two nucleic acids in solution, or a nucleic acid in solution to a nucleic acid attached to a solid support, *i.e.*, a filter. When one nucleic acid is on a solid support, a prehybridization step can be conducted prior to hybridization. Prehybridization can be carried out for at least about 1 hour, 3 hours or 10 hours in the same solution and at the same

-54-

temperature as the hybridization solution (without the complementary polynucleotide strand).

Appropriate stringency conditions are known to those skilled in the art or can be determined experimentally by the skilled artisan. See e.g. Ausubel et al., 1994; Sambrook & Russell, 2001; Agrawal, 1993; Tibanyenda et al., 1984; Ebel et al., 1992.

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The term "structural motif", when used in reference to a polypeptide, refers to a polypeptide that, although it can have different amino acid sequences, can result in a similar structure, wherein by structure is meant that the motif forms generally the same tertiary structure, or that certain amino acid residues within the motif, or alternatively their backbone or side chains (which can or can not include the $C\alpha$ atoms of the side chains) are positioned in a like relationship with respect to one another in the motif.

As applied to proteins, the term "substantial identity" means that two protein sequences, when optimally aligned, such as by the programs GAP or BESTFIT using default gap weights, typically share at least about 70 percent sequence identity, alternatively at least about 80, 85, 90, 95 percent sequence identity or more. In certain instances, residue positions that are not identical differ by conservative amino acid substitutions, which are described above.

As used herein, the term "substantially pure" refers to a polynucleotide or polypeptide that is substantially free of the sequences and molecules with which it is associated in its natural state, as well as from those molecules used in the isolation procedure. The term "substantially free" refers to that the sample is in one embodiment at least 50%, in another embodiment at least 70%, in another embodiment at least 80%, and in still another embodiment at least 90% free of the sequences and molecules with which is it associated in nature.

As used herein, the term "target cell" refers to a cell, into which it is desired to insert a nucleic acid sequence or polypeptide, or to otherwise effect a modification from conditions known to be present in the unmodified cell. A nucleic acid sequence introduced into a target cell can be of variable length.

-55-

Additionally, a nucleic acid sequence can enter a target cell as a component of a plasmid or other vector or as a naked sequence.

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The term "test compound" refers to a molecule to be tested by one or more screening method(s) as a putative modulator of a polypeptide of the invention or other biological entity or process. A test compound is usually not known to bind to a target of interest. The term "control test compound" refers to a compound known to bind to the target (i.e., a known agonist, antagonist, partial agonist or inverse agonist). The term "test compound" does not include a chemical added as a control condition that alters the function of the target to determine signal specificity in an assay. Such control chemicals or conditions include chemicals that 1) nonspecifically or substantially disrupt protein structure (i.e., denaturing agents (i.e., urea or guanidinium), chaotropic agents, sulfhydryl reagents (i.e., dithiothreitol and β-mercaptoethanol), and proteases), 2) generally inhibit cell metabolism (i.e., mitochondrial uncouplers) and 3) non-specifically disrupt electrostatic or hydrophobic interactions of a protein (i.e., high salt concentrations, or detergents at concentrations sufficient to non-specifically disrupt hydrophobic interactions). Further, the term "test compound" also does not include compounds known to be unsuitable for a therapeutic use for a particular indication due to toxicity of the subject. In certain embodiments, various predetermined concentrations of test compounds are used for screening such as 0.01 μM, 0.1 μM, 1.0 μM, and Examples of test compounds include, but are not limited to 10.0 μM. peptides, nucleic acids, carbohydrates, and small molecules. The term "novel test compound" refers to a test compound that is not in existence as of the filing date of this application. In certain assays using novel test compounds, the novel test compounds comprise at least about 50%, 75%, 85%, 90%, 95% or more of the test compounds used in the assay or in any particular trial of the assay.

The term "therapeutically effective amount" refers to that amount of a modulator, drug, or other molecule that is sufficient to effect treatment when administered to a subject in need of such treatment. The therapeutically effective amount will vary depending upon the subject and disease condition

-56-

being treated, the weight and age of the subject, the severity of the disease condition, the manner of administration and the like, which can readily be determined by one of ordinary skill in the art.

The term "transfection" means the introduction of a nucleic acid, *i.e.*, an expression vector, into a recipient cell, which in certain instances involves nucleic acid-mediated gene transfer. The term "transformation" refers to a process in which a cell's genotype is changed as a result of the cellular uptake of exogenous nucleic acid. For example, a transformed cell can express a recombinant form of a polypeptide of the invention or antisense expression can occur from the transferred gene so that the expression of a naturally occurring form of the gene is disrupted.

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The term "transgene" means a nucleic acid sequence, which is partly or entirely heterologous to a transgenic animal or cell into which it is introduced, or, is homologous to an endogenous gene of the transgenic animal or cell into which it is introduced, but which is designed to be inserted, or is inserted, into the animal's genome in such a way as to alter the genome of the cell into which it is inserted (*i.e.*, it is inserted at a location which differs from that of the natural gene or its insertion results in a knockout). A transgene can include one or more regulatory sequences and any other nucleic acids, such as introns, that can be necessary for optimal expression.

The term "transgenic animal" refers to any animal, for example, a mouse, rat or other non-human mammal, a bird or an amphibian, in which one or more of the cells of the animal contain heterologous nucleic acid introduced by way of human intervention, such as by transgenic techniques well known in the art. The nucleic acid is introduced into the cell, directly or indirectly, by way of deliberate genetic manipulation, such as by microinjection or by infection with a recombinant virus. The term genetic manipulation does not include classical cross-breeding, or *in vitro* fertilization, but rather is directed to the introduction of a recombinant DNA molecule. This molecule can be integrated within a chromosome, or it can be extrachromosomally replicating DNA. In the typical transgenic animals described herein, the transgene

causes cells to express a recombinant form of a protein. However, transgenic animals in which the recombinant gene is silent are also contemplated.

As used herein, the term "unit cell" refers to a basic parallelepiped shaped block. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal. Thus, the term "unit cell" refers to the fundamental portion of a crystal structure that is repeated infinitely by translation in three dimensions. A unit cell is characterized by three vectors, a, b, and c, not located in one plane, which form the edges of a parallelepiped. Angles α , β and γ define the angles between the vectors: angle α is the angle between vectors b and c; angle β is the angle between vectors a and c; and angle γ is the angle between vectors a and b. The entire volume of a crystal can be constructed by regular assembly of unit cells, each unit cell comprising a complete representation of the unit of pattern, the repetition of which builds up the crystal.

Unless otherwise indicated, all numbers expressing quantities of ingredients, reaction conditions, and so forth used in the specification and claims are to be understood as being modified in all instances by the term "about". Accordingly, unless indicated to the contrary, the numerical parameters set forth in this specification and attached claims are approximations that can vary depending upon the desired properties sought to be obtained by the present invention.

II. Description of Tables

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Table 1 is a table summarizing the crystal and data statistics obtained from the crystallized ligand-binding domain of CAR in complex with the ligand Compound 1. Data on the unit cell are presented, including data on the crystal space group, unit cell dimensions, molecules per asymmetric cell and crystal resolution.

Table 2 is a table of the atomic coordinate data obtained from X-ray diffraction from the ligand-binding domain of CAR in complex with the ligand Compound 1.

-58-

Table 3 is a table of the atomic structure coordinate data of the polyalanine model of the conserved vitamin D receptor ligand-binding domain.

III. General Considerations

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The present invention is applicable *mutatis mutandis* to all CARs, as discussed herein, based in part on the patterns of CAR structure and modulation that have emerged as a consequence of determining the three dimensional structure of CAR with bound ligand. Analysis and alignment of amino acid sequences, and X-ray and NMR structure determinations, have shown that nuclear receptors have a modular architecture with three main domains:

- 1) a variable amino-terminal domain;
- 2) a highly conserved DNA-binding domain (DBD); and
- 3) a less conserved carboxy-terminal ligand-binding domain (LBD).

In addition, nuclear receptors can have linker segments of variable length between these major domains. Sequence analysis and X-ray crystallography, including the work of the present invention, have confirmed that CARs, and indeed many NRs, also have the same general modular architecture, with the same three domains. The function of the CARs in human cells presumably requires all three domains in a single amino acid sequence. However, the modularity of the CARs permits different domains of each protein to separately accomplish certain functions.

Previous analysis of the nuclear receptors has revealed multiple discrete functional modules within the family that display generalized functional characteristics (for review see Beato et al., 1995; Kastner et al., 1995; Mangelsdorf & Evans, 1995; Tzukerman et al., 1994). A variable amino-terminal domain (A/B) is present that sometimes contains a strong and autonomous activation function (AF1), shown to be critical for cell and target gene specificity (Tora et al., 1988). A more carboxyl-terminal central region contains a DNA binding domain (DBD) characterized by two C4-type zinc fingers. The DBD binds to specific genomic response elements and thereby regulates the transcriptional activity of select genes containing the response

-59-

elements. At the distal carboxyl terminus, a ligand-binding domain (LBD) is present containing a highly conserved second transactivation function (AF2) that is important for hormone-dependent transcriptional transactivation (Lanz & Rusconi, 1994).

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Typically, the LBD forms a three-layered anti-parallel helical sandwich composed of 10-14 α helices and a β -sheet with 2-4 strands. The helices pack together so as to leave a binding pocket near the middle of the bundle, capped on one side by the β-sheet, and, in the "activated" state, capped on the other side by the AF2-helix. Comparison of apo, agonist-bound, and antagonist-bound nuclear receptor structures has led to a model for ligandinducible receptor action. In this model, the agonist (activating) ligands tend to hold the AF2 helix in a conformation where it "caps" the binding pocket. Antagonistic ligands usually shift the AF2 helix out of this "active" position. The AF2 helix can also shift into other conformations, positions, and orientations in the absence of ligand. Constitutively active receptors such as CAR should presumably utilize a similar mechanism of action, except that the AF2 helix adopts the "active" position, capping the ligand-binding pocket, even in the absence of ligand. Inverse agonists would presumably tend to shift the AF2 helix out of this "active" position, whereas superagonists would presumably tend to hold the AF2 helix more tightly in the active position. Central to the efficient ligand-induced transcriptional activation is the recruitment of co-regulator proteins - coactivators and co-repressors, which interact with the LBD and activate or repress transactivation, respectively (Moras & Gronemeyer, 1998; Weatherman et al., 1999; McKenna & O'Malley, 2000). In general, the conformational changes described above involving the AF2 helix cause changes in the affinity of the LBD for co-repressors versus coactivators. The binding of an agonist results in a dissociation of corepressors and brings the AF2 into a context where it can interact with transcriptional coactivators. Likewise, an antagonist would be expected to disrupt the binding of coactivators.

Sequences that function in nuclear localization, receptor dimerization, and interaction with heat-shock proteins (Gronemeyer & Laudet, 1995) are

-60-

also present within the nuclear receptor substructure. Through the coordinated action of these separate functional domains, nuclear receptor activation by ligand culminates in modulation of target gene expression through DNA interactions (Tsai & O'Malley, 1994) or in certain other cases through cross-talk with other cell signaling pathways (Stein & Yang, 1995; Paech et al., 1998). In short, a ligand alters nuclear receptor function by altering the conformation of the receptor and consequently the constellation of protein-protein interactions in which the receptor is engaged (Freedman, 1999).

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Some of the functions of a domain within the full-length receptor are preserved when that particular domain is isolated from the remainder of the protein. Using conventional protein chemistry techniques, a modular domain can sometimes be separated from the parent protein. Using conventional molecular biology techniques, each domain can usually be separately expressed with its original function intact or, as discussed herein below, chimeras comprising two different proteins can be constructed, wherein the chimeras retain the properties of the individual functional domains of the respective nuclear receptors from which the chimeras were generated.

The LBD is the second most highly conserved domain in these 3 domains. As its name suggests, the LBD binds ligands. With many nuclear receptors binding of the ligand can induce a conformational change in the LBD that can, in turn, increase or decrease transcription of certain target genes. The LBD also participates in other functions, including dimerization and nuclear translocation.

X-ray structures have shown that most nuclear receptor LBDs adopt the same general folding pattern. This fold includes 10-12 alpha helices arranged in a bundle, together with several beta-strands, additional alpha helices and linking segments. The major alpha helices and beta-strands have been numbered differently in different publications. The present disclosure follows the numbering scheme of Nolte *et al.*, 1998, where the major alphahelices and beta-strands in PPARγ were designated sequentially through the amino acid sequence as H1, H2, S1, H2', H3, H3', H4, H5, S2, S3, S4, H6,

H7, H8, H9, H10 and HAF. The alpha helix at the C-terminal end, HAF, is also called "helix-AF", "helix-AF2" the "AF2 helix" or "helix-12". Most, but not all, of these alpha helices and beta-strands are observed in the structure of CAR. An additional helix, designated here as "helix-X", is observed in the structure of CAR bound to Compound 1 on the C-terminal side of H10.

As described herein, the LBD of a CAR can be expressed, crystallized, its three dimensional structure determined with a ligand bound as disclosed in the present invention, and computational methods can be used to design ligands to its LBD.

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IV. Synthesis of CAR Ligands and Intermediates

IV.A. Compound 1 - An Embodiment of a Synthetic CAR Ligand

In one embodiment, the present invention provides compounds of Compound 1 (Formula (A) below) and tautomeric forms, pharmaceutically acceptable salts and solvates thereof:

IV.B. Synthesis of Compound 1 and Intermediates

Compound 1, which was co-crystallized with the CAR LBD in the present invention, can be prepared as described in Example 6 and shown in

Figure 7. Briefly, a solution of 3-fluoro-4-nitrobenzoic acid in anhydrous N,Ndimethylformamide was treated with [O-(7-azabenzotriazol-1-yl)-1,1,3,3tetramethyluronium hexafluorophosphate] followed by N.Ndiisopropylethylamine. After shaking for 5 minutes, the mixture was added to polystyrene Rink amide AM resin, and the reaction was rotated at 25°C for 18 hours. The reaction solution was drained, and the resin was washed with N,N-dimethylformamide, dichloromethane, methanol, and dichloromethane. The dried resin was treated with a 0.5 M phenethylamine in Nmethylpyrrolidinone solution and incubated with rotation for 15 hours at 70°C. The reaction was cooled to room temperature, drained, and the resin was washed as before. The resin was then treated with a 2.0 M SnCl₂•dihydrate in N-methylpyrrolidinone solution for 24 hours at 25°C with rotation. reaction was drained and the resin washed with 30% ethylenediamine. N.Ndimethylformamide, dichloromethane, methanol, and dichloromethane. The dried diamine resin was treated with a 0.5 M benzyhydryl isothiocyanate in Nmethylpyrrolidinone solution and a 1.0 M diisopropylcarbodiimide in Nmethylpyrrolidinone solution at 80°C with rotation. After 24 hours, the reaction was cooled to 25°C, drained, and the resin was washed with N,Ndimethylformamide, dichloromethane, methanol, and dichloromethane. The resin was then treated with 95:5 TFA:H₂O and rotated at 25°C for 3 hours. The resin was drained and washed with dichloromethane. The filtrate was concentrated in vacuo to give an oil. The oil was redissolved in dichloromethane and the solution was washed twice with saturated sodium bicarbonate. The organic layer was dried (Na₂SO₄), filtered, and concentrated in vacuo. The crude product was triturated with Et₂O/hexanes, and the solid was collected by filtration to give Compound 1 as an off-white solid.

V. Production of CAR Polypeptides

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The native and mutated CAR polypeptides, and fragments thereof, of the present invention can be chemically synthesized in whole or part using techniques that are well known in the art (see e.g., Creighton, 1983, incorporated herein in its entirety). Alternatively, methods which are well

-63-

known to those skilled in the art can be used to construct expression vectors containing a partial or the entire native or mutated CAR polypeptide coding sequence and appropriate transcriptional/translational control signals. These methods include *in vitro* recombinant DNA techniques, synthetic techniques, and *in vivo* recombination/genetic recombination (see e.g., the techniques described throughout Sambrook & Russell, 2001, and Ausubel et al., 1994, both incorporated herein in their entirety).

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A variety of host-expression vector systems can be utilized to express a CAR coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing a CAR coding sequence; yeast transformed with recombinant yeast expression vectors containing a CAR coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g., baculovirus) containing a CAR coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosaic virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing a CAR coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities.

Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, can be used in the expression vector. For example, when cloning in bacterial systems, inducible promoters such as pL of bacteriophage λ , plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like can be used. When cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter can be used. When cloning in plant cell systems, promoters derived from the genome of plant cells, such as heat shock promoters; the promoter for the small subunit of ribulose bisphosphate carboxylase (RUBISCO); the promoter for the chlorophyll a/b binding protein; or from plant viruses (e.g., the 35S RNA promoter of CaMV; the coat protein promoter of TMV) can be used. When cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein

-64-

promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) can be used.

In each of these systems, one of ordinary skill in the art will appreciate that other promoters can be used, and as such, the list presented is not intended to be exhaustive.

VI. Analysis of Protein Properties

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VI.A. Analysis of Proteins by X-ray Crystallography Generally

VI.A.1. X-ray Structure Determination

Exemplary methods for obtaining the three dimensional structure of the crystalline form of a molecule or complex are described herein and, in view of this specification, variations on these methods will be apparent to those skilled in the art (see Ducruix & Geige, 1992).

A variety of methods involving X-ray crystallography are contemplated by the present invention. For example, the present invention contemplates producing a crystallized polypeptide of the invention, or a fragment thereof, by: (a) introducing into a host cell an expression vector comprising a nucleic acid encoding for a polypeptide of the invention, or a fragment thereof; (b) culturing the host cell in a cell culture medium to express the polypeptide or fragment; (c) isolating the polypeptide or fragment from the cell culture; and (d) crystallizing the polypeptide or fragment thereof. Alternatively, the present invention contemplates determining the three dimensional structure of a crystallized polypeptide of the invention, or a fragment thereof, by: (a) crystallizing a polypeptide of the invention, or a fragment thereof, such that the crystals will diffract X-rays to a resolution of 2.5 Å or better; and (b) analyzing the polypeptide or fragment by X-ray diffraction to determine the three-dimensional structure of the crystallized polypeptide.

X-ray crystallography techniques generally require that the protein molecules be available in the form of a crystal. Crystals can be grown from a solution containing a purified polypeptide of the invention, or a fragment thereof (i.e., a ligand-binding domain), by a variety of conventional processes. These processes include, for example, batch, liquid, bridge, dialysis, and

vapor diffusion (i.e., hanging drop or sitting drop methods). See e.g., McPherson, 1982; McPherson, 1990; Webe, 1991.

In certain embodiments, native crystals of the invention can be grown by adding precipitants to the concentrated solution of the polypeptide. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water can be removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

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The formation of crystals is dependent on a number of different parameters, including pH, temperature, protein concentration, the nature of the solvent and precipitant, as well as the presence of added ions or ligands to the protein. In addition, the sequence of the polypeptide being crystallized will have a significant affect on the success of obtaining crystals. Many routine crystallization experiments can be needed to screen all these parameters for the few combinations that might give crystal suitable for X-ray diffraction analysis. See e.g., Jancarik & Kim, 1991.

Crystallization robots can automate and speed up the work of reproducibly setting up large number of crystallization experiments. Once some suitable set of conditions for growing the crystal are found, variations of the condition can be systematically screened in order to find the set of conditions which allows the growth of sufficiently large, single, well ordered crystals. In certain instances, a polypeptide of the invention is co-crystallized with a ligand: in one embodiment, Compound 1.

A number of methods are available to produce suitable radiation for X-ray diffraction. For example, X-ray beams can be produced by synchrotron rings where electrons (or positrons) are accelerated through an electromagnetic field while traveling at close to the speed of light. Because the admitted wavelength can also be controlled, synchrotrons can be used as a tunable X-ray source (Hendrickson, 2000). For less conventional Laue diffraction studies, polychromatic X-rays covering a broad wavelength window are used to observe many diffraction intensities simultaneously (Stoddard,

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1998). Neutrons can also be used for solving protein crystal structures (Gutberlet et al., 2001).

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Before data collection commences, a protein crystal can be frozen to protect it from radiation damage. A number of different cryo-protectants can be used to assist in freezing the crystal, such as methyl pentanediol (MPD), isopropanol, ethylene glycol, glycerol, formate, citrate, mineral oil, or a low-molecular-weight polyethylene glycol (PEG). The present invention contemplates a composition comprising a polypeptide of the invention and a cryo-protectant. As an alternative to freezing the crystal, the crystal can also be used for diffraction experiments performed at temperatures above the freezing point of the solution. In these instances, the crystal can be protected from desiccation by placing it in a narrow capillary of a suitable material (generally glass or quartz) with some of the crystal growth solution included in order to maintain vapor pressure.

X-ray diffraction results can be recorded by a number of ways known to one of skill in the art. Examples of area electronic detectors include charge coupled device detectors, multi-wire area detectors, and phosphoimager detectors (Amemiya, 1997; Westbrook & Naday, 1997; Kahn & Fourme, 1997).

A suitable system for laboratory data collection might include a Bruker AXS Proteum R system, equipped with a copper rotating anode source, Confocal MAX-FLUXTM optics and a SMART 6000 charge coupled device detector. Collection of X-ray diffraction patterns is well known to those skilled in the art (see e.g. Ducruix & Geige, 1992).

The theory behind diffraction by a crystal upon exposure to X-rays is well known. Because phase information is not directly measured in the diffraction experiment and is needed to reconstruct the electron density map, methods that can recover this missing information are required. One method of solving structures *ab initio* is the real/reciprocal space cycling technique. Suitable real/reciprocal space cycling search programs include Shake-and-Bake (Miller *et al.*, 1993; Weeks *et al.*, 1994).

Other methods for deriving phases might also be needed. These techniques generally rely on the idea that if two or more measurements of the same reflection are made where strong, measurable, differences are attributable to the characteristics of a small subset of the atoms alone, then the contributions of other atoms can be, to a first approximation, ignored, and the positions of these atoms can be determined from the difference in scattering by one of the above techniques. Knowing the position and scattering characteristics of those atoms, one can calculate what phase the overall scattering must have had to produce the observed differences.

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One version of this technique is the isomorphous replacement technique, which requires the introduction of new, well ordered, X-ray scatterers into the crystal. These additions are usually heavy metal atoms, (so that they make a significant difference in the diffraction pattern); and if the additions do not change the structure of the molecule or of the crystal cell, the resulting crystals should be isomorphous. Isomorphous replacement experiments are usually performed by diffusing different heavy-metal metals into the channels of a pre-existing protein crystal. Growing the crystal from protein that has been soaked in the heavy atom is also possible (Petsko, 1985). Alternatively, the heavy atom can also be reactive and attached covalently to exposed amino acid side chains (such as the sulfur atom of cysteine) or it can be associated through non-covalent interactions. It is sometimes possible to replace endogenous light metals in metallo-proteins with heavier ones, i.e., zinc by mercury, or calcium by samarium (Petsko, 1985). Exemplary sources for such heavy compounds include, but are not limited to, sodium bromide, sodium selenate, trimethyl lead acetate, mercuric chloride, methyl mercury acetate, platinum tetracyanide, platinum tetrachloride, nickel chloride, and europium chloride.

A second technique for generating differences in scattering involves the phenomenon of anomalous scattering. X-rays that cause the displacement of an electron in an inner shell to a higher shell are subsequently rescattered, but there is a time lag that shows up as a phase delay. This phase delay is observed as a (generally quite small) difference in

-68-

intensity between reflections known as Friedel mates that would be identical if no anomalous scattering were present. A second effect related to this phenomenon is that differences in the intensity of scattering of a given atom will vary in a wavelength-dependent manner, giving rise to what are known as dispersive differences. In principle, anomalous scattering occurs with all atoms, but the effect is strongest with heavy atoms, and can be maximized by using X-rays at a wavelength where the energy is equal to the difference in energy between shells. The technique therefore requires the incorporation of some heavy atom much as is needed for isomorphous replacement, although for anomalous scattering a wider variety of atoms are suitable, including lighter metal atoms (copper, zinc, iron) in metallo-proteins. One method for preparing a protein for anomalous scattering involves replacing the methionine residues in whole or in part with selenium-containing selenomethionine. Soaking with halide salts such as bromides and other non-reactive ions can also be effective (Dauter et al., 2001).

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In another process, known as multiple anomalous scattering or MAD, two to four suitable wavelengths of data are collected. (Hendrickson & Ogata, 1997). Phasing by various combinations of single and multiple isomorphous and anomalous scattering are possible too. For example, SIRAS (single isomorphous replacement with anomalous scattering) utilizes both the isomorphous and anomalous differences for one derivative to derive phases. More traditionally, several different heavy atoms are soaked into different crystals to get sufficient phase information from isomorphous differences while ignoring anomalous scattering, in the technique known as multiple isomorphous replacement (MIR) (Petsko, 1985).

Additional restraints on the phases can be derived from density modification techniques. These techniques use either generally known features of electron density distribution or known facts about that particular crystal to improve the phases. For example, because protein regions of the crystal scatter more strongly than solvent regions, solvent flattening/flipping can be used to adjust phases to make solvent density a uniform flat value (Zhang et al., 1997). If more than one molecule of the protein is present in the

-69-

asymmetric unit, the fact that the different molecules should be virtually identical can be exploited to further reduce phase error using non-crystallographic symmetry averaging (Villieux & Read, 1997). Suitable programs for performing these processes include DM and other programs of the CCP4 suite (Collaborative Computational Project, 1994) and CNX.

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The unit cell dimensions, symmetry, vector amplitude and derived phase information can be used in a Fourier transform function to calculate the electron density in the unit cell, *i.e.*, to generate an experimental electron density map. This can be accomplished using programs of the CNX or CCP4 packages. The resolution is measured in Ångstrom (Å) units, and is closely related to how far apart two objects need to be before they can be reliably distinguished. The smaller this number is, the higher the resolution and therefore the greater the amount of detail that can be seen. In alternative embodiments, crystals of the invention diffract X-rays to a resolution of better than about 4.0, 3.5, 3.0, 2.5, 2.0, 1.5, 1.0, 0.5 Å, or better.

As used herein, the term "modeling" includes the quantitative and qualitative analysis of molecular structure and/or function based on atomic structural information and interaction models. The term "modeling" includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and other structure-based constraint models.

Model building can be accomplished by either the crystallographer using a computer graphics program such as TURBO or O (Jones *et al.*, 1991) or, under suitable circumstances, by using a fully automated model building program, such as wARP (Perrakis *et al.*, 1999) or MAID (Levitt, 2001). This structure can be used to calculate model-derived diffraction amplitudes and phases. The model-derived and experimental diffraction amplitudes can be compared and the agreement between them can be described by a parameter referred to as R-factor. A high degree of correlation in the amplitudes corresponds to a low R-factor value, with 0.0 representing exact agreement and 0.59 representing a completely random structure. Because the R-factor can be lowered by introducing more free parameters into the model, an

unbiased, cross-correlated version of the R-factor known as the R-free gives a more objective measure of model quality. For the calculation of this parameter a subset of reflections (generally around 10%) are set aside at the beginning of the refinement and not used as part of the refinement target. These reflections are then compared to those predicted by the model (Kleywegt & Brunger, 1996).

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The model can be improved using computer programs that maximize the probability that the observed data was produced from the predicted model. while simultaneously optimizing the model geometry. For example, the CNX program can be used for model refinement, as can the XPLOR program (Murshudov et al., 1997). In order to maximize the convergence radius of refinement, simulated annealing refinement using torsion angle dynamics can be employed in order to reduce the degrees of freedom of motion of the model (Adams et al., 1997). Where experimental phase information is available (i.e., where MAD data was collected) Hendrickson-Lattman phase probability targets can be employed. Isotropic or anisotropic domain, group or individual temperature factor refinement, can be used to model variance of the atomic position from its mean. Well-defined peaks of electron density not attributable to protein atoms are generally modeled as water molecules. Water molecules can be found by manual inspection of electron density maps, or with automatic water picking routines. Additional small molecules. including ions, cofactors, buffer molecules, or substrates can be included in the model if sufficiently unambiguous electron density is observed in a map.

In general, the R-free is rarely as low as 0.15 and can be as high as 0.35 or greater for a reasonably well-determined protein structure. The residual difference is a consequence of approximations in the model (inadequate modeling of residual structure in the solvent, modeling atoms as isotropic Gaussian spheres, assuming all molecules are identical rather than having a set of discrete conformers, etc.) and errors in the data (Lattman, 1996). In refined structures at high resolution, there are usually no major errors in the orientation of individual residues, and the estimated errors in atomic positions are usually around 0.1 - 0.2 up to 0.3 Å.

The three dimensional structure of a new crystal can be modeled using molecular replacement. The term "molecular replacement" refers to a method that involves generating a preliminary model of a molecule or complex whose structure coordinates are unknown, by orienting and positioning a molecule whose structure coordinates are known within the unit cell of the unknown crystal, so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal (Lattman, 1985; Rossmann, 1972).

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Commonly used computer software packages for molecular replacement are CNX, X-PLOR (Brunger 1992, *Nature* 355: 472-475), AMORE (Navaza, 1994, *Acta Crystallogr.* A50:157-163), the CCP4 package, the MERLOT package (Fitzgerald, 1988) and XTALVIEW (McCree *et al.*, 1992). The quality of the model can be analyzed using a program such as PROCHECK or 3D-Profiler (Laskowski *et al.*, 1993; Luthy *et al.*, 1992; Bowie *et al.*, 1991).

Homology modeling (also known as comparative modeling or knowledge-based modeling) methods can also be used to develop a three dimensional model from a polypeptide sequence based on the structures of known proteins. The method utilizes a computer model of a known protein, a computer representation of the amino acid sequence of the polypeptide with an unknown structure, and standard computer representations of the structures of amino acids. This method is well known to those skilled in the art (Greer, 1985; Blundell et al., 1988; Knighton et al., 1992). Computer programs that can be used in homology modeling are QUANTA and the Homology module in the Insight II modeling package distributed by Molecular Simulations Inc. (now part of Accelrys Inc., San Diego, California, United States of America), or MODELLER (Rockefeller University, New York, New York, United States of America). These computer programs can also be used

-72-

for computational loop modeling techniques. See also Tosatto et al., 2002; Fiser et al., 2000.

Once a homology model has been generated it is analyzed to determine its correctness. A computer program available to assist in this analysis is the Protein Health module in QUANTA that provides a variety of tests. Other programs that provide structure analysis along with output include PROCHECK and 3D-Profiler (Luthy et al., 1992; Bowie et al., 1991). Once any irregularities have been resolved, the entire structure can be further refined.

Other molecular modeling techniques can also be employed in accordance with this invention. See e.g., Cohen et al., 1990; Navia & Murcko, 1992.

Under suitable circumstances, the entire process of solving a crystal structure can be accomplished in an automated fashion by a system such as ELVES (http://ucxray.berkeley.edu/~jamesh/elves/index.html) with little or no user intervention.

VI.A.2. X-ray Structure

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The present invention provides methods for determining some or all of the structural coordinates for amino acids of a polypeptide of the invention, or a complex thereof.

In another aspect, the present invention provides methods for identifying a druggable region of a polypeptide of the invention. For example, one such method includes: (a) obtaining crystals of a polypeptide of the invention or a fragment thereof such that the three dimensional structure of the crystallized protein can be determined to a resolution of 2.5 Å or better; (b) determining the three dimensional structure of the crystallized polypeptide or fragment using X-ray diffraction; and (c) identifying a druggable region of a polypeptide of the invention based on the three-dimensional structure of the polypeptide or fragment.

A three dimensional structure of a molecule or complex can be described by the set of atoms that best predict the observed diffraction data

(that is, which possesses a minimal R value). Files can be created for the structure that defines each atom by its chemical identity, spatial coordinates in three dimensions, root mean squared deviation from the mean observed position and fractional occupancy of the observed position.

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Those of skill in the art understand that a set of structure coordinates for a protein, complex, or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates can have little affect on overall shape. Such variations in coordinates can be generated because of mathematical manipulations of the structure coordinates. For example, structure coordinates could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates. integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above. Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal, could also yield variations in structure coordinates. Such slight variations in the individual coordinates will have little affect on overall shape. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be structurally equivalent. It should be noted that slight variations in individual structure coordinates of a polypeptide of the invention or a complex thereof would not be expected to significantly alter the nature of modulators that could associate with a druggable region thereof. Thus, for example, a modulator that bound to the active site of a polypeptide of the invention would also be expected to bind to or interfere with another active site whose structure coordinates define a shape that falls within the acceptable error.

A crystal structure of the present invention can be used to make a structural or computer model of the polypeptide, complex, or portion thereof. A model can represent the secondary, tertiary, and/or quaternary structure of

-74-

the polypeptide, complex, or portion. The configurations of points in space derived from structure coordinates according to the invention can be visualized as, for example, a holographic image, a stereodiagram, a model, or a computer-displayed image, and the invention thus includes such images, diagrams, or models.

VI.A.3. Structural Equivalents

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Various computational analyses can be used to determine whether a molecule or the active site portion thereof is structurally equivalent with respect to its three-dimensional structure, to all or part of a structure of a polypeptide of the invention or a portion thereof.

For the purpose of this invention, any molecule or complex or portion thereof, that has a root mean square deviation of conserved residue backbone atoms (N, $C\alpha$, C, O) of less than about 1.75 Å, when superimposed on the relevant backbone atoms described by the reference structure coordinates of a polypeptide of the invention, is considered "structurally equivalent" to the reference molecule. That is to say, the crystal structures of those portions of the two molecules are substantially identical, within acceptable error. Alternatively, the root mean square deviation can be is less than about 1.50, 1.40, 1.25, 1.0, 0.75, 0.5 or 0.35 Å.

The term "root mean square deviation" is understood in the art and means the square root of the arithmetic mean of the squares of the deviations. It is a way to express the deviation or variation from a trend or object.

In another aspect, the present invention provides a scalable three-dimensional configuration of points, at least a portion of said points, and preferably all of said points, derived from structural coordinates of at least a portion of a polypeptide of the invention and having a root mean square deviation from the structure coordinates of the polypeptide of the invention of less than 1.50, 1.40, 1.25, 1.0, 0.75, 0.5 or 0.35 Å. In certain embodiments, the portion of a polypeptide of the invention is 25%, 33%, 50%, 66%, 75%,

-75-

85%, 90%, or 95% or more of the amino acid residues contained in the polypeptide.

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In another aspect, the present invention provides a molecule or complex including a druggable region of a polypeptide of the invention, the druggable region being defined by a set of points having a root mean square deviation of less than about 1.75 Å from the structural coordinates for points representing (a) the backbone atoms of the amino acids contained in a druggable region of a polypeptide of the invention, (b) the side chain atoms (and optionally the $C\alpha$ atoms) of the amino acids contained in such druggable region, or (c) all the atoms of the amino acids contained in such druggable region. In certain embodiments, only a portion of the amino acids of a druggable region can be included in the set of points, such as 25%, 33%, 50%, 66%, 75%, 85%, 90% or 95% or more of the amino acid residues contained in the druggable region. In certain embodiments, the root mean square deviation can be less than 1.50, 1.40, 1.25, 1.0, 0.75, 0.5, or 0.35 Å. In still other embodiments, instead of a druggable region, a stable domain, fragment, or structural motif is used in place of a druggable region.

VI.A.4. Machine Displays and Machine Readable Storage Media

The invention provides a machine-readable storage medium including a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of any of the molecules or complexes, or portions thereof, of this invention. In another embodiment, the graphical three-dimensional representation of such molecule, complex, or portion thereof includes the root mean square deviation of certain atoms of such molecule by a specified amount, such as the backbone atoms by less than 1.5 Å. In another embodiment, a structural equivalent of such molecule, complex, or portion thereof, can be displayed. In another embodiment, the portion can include a druggable region of the polypeptide of the invention.

According to one embodiment, the invention provides a computer for determining at least a portion of the structure coordinates corresponding to X-

ray diffraction data obtained from a molecule or complex, wherein said computer includes: (a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structural coordinates of a polypeptide of the invention; (b) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises X-ray diffraction data from said molecule or complex; (c) a working memory for storing instructions for processing said machine-readable data of (a) and (b); (d) a central-processing unit coupled to said working memory and to said machine-readable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structure coordinates; and (e) a display coupled to said central-processing unit for displaying said structure coordinates of said molecule or complex. In certain embodiments, the structural coordinates displayed are structurally equivalent to the structural coordinates of a polypeptide of the invention.

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In an alternative embodiment, the machine-readable data storage medium includes a data storage material encoded with a first set of machine readable data which includes the Fourier transform of the structure coordinates of a polypeptide of the invention or a portion thereof, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine readable data including the X-ray diffraction pattern of a molecule or complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

For example, a system for reading a data storage medium can include a computer including a central processing unit (CPU), a working memory which can be, i.e., random access memory (RAM) or "core" memory, mass storage memory (such as one or more disk drives or CD-ROM drives), one or more display devices (i.e., cathode-ray tube ("CRT") displays, light emitting diode (LED) displays, liquid crystal displays (LCDs), electroluminescent displays, vacuum fluorescent displays, field emission displays (FEDs), plasma

displays, projection panels, etc.), one or more user input devices (*i.e.*, keyboards, microphones, mice, touch screens, etc.), one or more input lines, and one or more output lines, all of which are interconnected by a conventional bidirectional system bus. The system can be a stand-alone computer, or can be networked (*i.e.*, through local area networks, wide area networks, intranets, extranets, or the internet) to other systems (*i.e.*, computers, hosts, servers, etc.). The system can also include additional computer controlled devices such as consumer electronics and appliances.

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Input hardware can be coupled to the computer by input lines and can be implemented in a variety of ways. Machine-readable data of this invention can be inputted via the use of a modern or moderns connected by a telephone line or dedicated data line. Alternatively or additionally, the input hardware can include CD-ROM drives or disk drives. In conjunction with a display terminal, a keyboard can also be used as an input device.

Output hardware can be coupled to the computer by output lines and can similarly be implemented by conventional devices. By way of example, the output hardware can include a display device for displaying a graphical representation of an active site of this invention using a program such as QUANTA as described herein. Output hardware might also include a printer, so that hard copy output can be produced, or a disk drive, to store system output for later use.

In operation, a CPU coordinates the use of the various input and output devices, coordinates data accesses from mass storage devices, accesses to and from working memory, and determines the sequence of data processing steps. A number of programs can be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. References to components of the hardware system are included as appropriate throughout the following description of the data storage medium.

Machine-readable storage devices useful in the present invention include, but are not limited to, magnetic devices, electrical devices, optical devices, and combinations thereof. Examples of such data storage devices

-78-

include, but are not limited to, hard disk devices, CD devices, digital video disk devices, floppy disk devices, removable hard disk devices, magneto-optic disk devices, magnetic tape devices, flash memory devices, bubble memory devices, holographic storage devices, and any other mass storage peripheral device. It should be understood that these storage devices include necessary hardware (i.e., drives, controllers, power supplies, etc.) as well as any necessary media (i.e., disks, flash cards, etc.) to enable the storage of data.

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In one embodiment, the present invention contemplates a computer readable storage medium comprising structural data, wherein the data include the identity and three-dimensional coordinates of a polypeptide of the invention or portion thereof. In another aspect, the present invention contemplates a database comprising the identity and three-dimensional coordinates of a polypeptide of the invention or a portion thereof. Alternatively, the present invention contemplates a database comprising a portion or all of the atomic coordinates of a polypeptide of the invention or portion thereof.

VI.A.5. Structurally Similar Molecules and Complexes

Structural coordinates for a polypeptide of the invention can be used to aid in obtaining structural information about another molecule or complex. This method of the invention allows determination of at least a portion of the three-dimensional structure of molecules or molecular complexes that contain one or more structural features that are similar to structural features of a polypeptide of the invention. Similar structural features can include, for example, regions of amino acid identity, conserved active site or binding site motifs, and similarly arranged secondary structural elements (*i.e.*, α helices and β sheets). Many of the methods described above for determining the structure of a polypeptide of the invention can be used for this purpose as well.

For the present invention, a "structural homolog" is a polypeptide that contains one or more amino acid substitutions, deletions, additions, or rearrangements with respect to the amino acid sequence of SEQ ID NOs: 2

-79-

or 4 or other polypeptide of the invention, but that, when folded into its native conformation, exhibits or is reasonably expected to exhibit at least a portion of the tertiary (three-dimensional) structure of the polypeptide encoded by SEQ ID NOs: 2 or 4 or such other polypeptide of the invention. For example, structurally homologous molecules can contain deletions or additions of one or more contiguous or noncontiguous amino acids, such as a loop or a domain. Structurally homologous molecules also include modified polypeptide molecules that have been chemically or enzymatically derivatized at one or more constituent amino acids, including side chain modifications, backbone modifications, and N- and C-terminal modifications including acetylation, hydroxylation, methylation, amidation, and the attachment of carbohydrate or lipid moieties, cofactors, and the like.

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By using molecular replacement, all or part of the structure coordinates of a polypeptide of the invention can be used to determine the structure of a crystallized molecule or complex whose structure is unknown more quickly and efficiently than attempting to determine such information *ab initio*. For example, in one embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or complex whose structure is unknown including: (a) crystallizing the molecule or complex of unknown structure; (b) generating an X-ray diffraction pattern from said crystallized molecule or complex; and (c) applying at least a portion of the structure coordinates for a polypeptide of the invention to the X-ray diffraction pattern to generate a three-dimensional electron density map of the molecule or complex whose structure is unknown.

In another aspect, the present invention provides a method for generating a preliminary model of a molecule or complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of a polypeptide of the invention within the unit cell of the crystal of the unknown molecule or complex so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or complex whose structure is unknown.

Structural information about a portion of any crystallized molecule or complex that is sufficiently structurally similar to a portion of a polypeptide of

-80-

the invention can be resolved by this method. In addition to a molecule that shares one or more structural features with a polypeptide of the invention, a molecule that has similar bloactivity, such as the same catalytic activity, substrate specificity or ligand-binding activity as a polypeptide of the invention, can also be sufficiently structurally similar to a polypeptide of the invention to permit use of the structure coordinates for a polypeptide of the invention to solve its crystal structure.

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In another aspect, the method of molecular replacement is utilized to obtain structural information about a complex containing a polypeptide of the invention, such as a complex between a modulator and a polypeptide of the invention (or a domain, fragment, ortholog, homolog etc. thereof). In certain instances, the complex includes a polypeptide of the invention (or a domain, fragment, ortholog, homolog etc. thereof) co-complexed with a modulator. For example, in one embodiment, the present invention contemplates a method for making a crystallized complex comprising a polypeptide of the invention, or a fragment thereof, and a compound having a molecular weight of less than 5 kDa, the method comprising: (a) crystallizing a polypeptide of the invention such that the crystals will diffract X-rays to a resolution of 2.5 Å or better; and (b) soaking the crystal in a solution comprising the compound having a molecular weight of less than 5 kDa, thereby producing a crystallized complex comprising the polypeptide and the compound.

Using homology modeling, a computer model of a structural homolog or other polypeptide can be built or refined without crystallizing the molecule. For example, in another aspect, the present invention provides a computer-assisted method for homology modeling a structural homolog of a polypeptide of the invention including: aligning the amino acid sequence of a known or suspected structural homolog with the amino acid sequence of a polypeptide of the invention and incorporating the sequence of the homolog into a model of a polypeptide of the invention derived from atomic structure coordinates to yield a preliminary model of the homolog; subjecting the preliminary model to energy minimization to yield an energy minimized model; remodeling regions

-81-

of the energy minimized model where stereochemistry restraints are violated to yield a final model of the homolog.

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In another embodiment, the present invention contemplates a method for determining the crystal structure of a homolog of a polypeptide having SEQ ID NO: 2 or SEQ ID NO: 4, or equivalent thereof, the method comprising: (a) providing the three dimensional structure of a crystallized polypeptide having SEQ ID NO: 2 or SEQ ID NO: 4, or a fragment thereof; (b) obtaining crystals of a homologous polypeptide comprising an amino acid sequence that is at least 80% identical to the amino acid sequence set forth in SEQ ID NO: 2 or SEQ ID NO: 4 such that the three dimensional structure of the crystallized homologous polypeptide can be determined to a resolution of 2.5 Å or better; and (c) determining the three dimensional structure of the crystallized homologous polypeptide by X-ray crystallography based on the atomic coordinates of the three dimensional structure provided in step (a). In certain instances of the foregoing method, the atomic coordinates for the homologous polypeptide have a root mean square deviation from the backbone atoms of the polypeptide having SEQ ID NO: 2 or SEQ ID NO: 4, or a fragment thereof, of not more than 1.5 Å for all backbone atoms shared in common with the homologous polypeptide and the polypeptide having SEQ ID NO: 2 or SEQ ID NO: 4, or a fragment thereof.

In another aspect, the present invention provides a method for building a model for the activated conformation of CAR, using the repressed structure of Table 2 as a template. In one embodiment, the method comprises: (a) taking the coordinates for residues 107 to 332 directly from Table 2, effectively assuming that the conformation of this portion of CAR is similar or identical in the activated and repressed states; (b) rotating and translating an X-ray structure of VDR, the Vitamin-D receptor, so as to superimpose its core backbone atoms onto corresponding atoms from CAR; (c) combining the superimposed VDR AF2 helix, residues 416-423, with residues 107-332 from the initial CAR model of step (a), to serve as the starting model for residues 107-332 and 341-348 of the CAR protein in the activated conformation; (d) computationally mutating Val418, Leu419, Val421, Phe422 and Gly423 in the

-82-

transplanted VDR AF2 helix to the corresponding amino acid types in the CAR AF2 helix, which are Leu343, Gln344, Ile346, Cys347 and Ser348, respectively; and (e) adjusting the conformations of the mutated amino acid side-chains in the AF2 helix of the CAR model, residues 343, 344, and 346-348, to avoid overlaps by using either manual manipulation within molecular graphics programs or conformational search and energy minimization. In one embodiment, the method further comprises modeling the CAR AF2 linker region, residues 333-340, by using a computational loop modeling technique, recognizing that the calculated linker conformation would probably deviate considerably from the actual linker conformation.

VII. Formation of CAR Ligand-Binding Domain-Ligand Crystals

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The present invention provides crystals of CAR LBD in complex with the ligand. The crystals were obtained using the methodology disclosed in the Examples. The CAR LBD-ligand crystals, which can be native or derivative crystals, have orthorhombic unit cells (an orthorhombic unit cell is a unit cell wherein $a \neq b \neq c$, and wherein $\alpha = \beta = \gamma = 90^{\circ}$) and space group symmetry P2₁2₁2₁. There are four CAR LBD molecules in the asymmetric unit. In this CAR crystalline form, the unit cell has dimensions of a = 83.0 Å, b = 116.8 Å, c = 131.9 Å, and $\alpha = \beta = \gamma = 90^{\circ}$. This crystal form can be formed in a crystallization reservoir comprising 1 μ l of the protein-ligand solutions disclosed herein, and 1 μ l of well buffer (e.g. 100-400 mM sodium potassium tartrate, pH 7.1-7.4).

The native and derivative co-crystals comprising a CAR LBD and a ligand disclosed in the present invention can be obtained by a variety of techniques, including batch, liquid bridge, dialysis, vapor diffusion and hanging drop methods (see e.g., McPherson, 1982; McPherson, 1990; Weber, 1991). In one embodiment, the vapor diffusion and hanging drop methods are used for the crystallization of CAR polypeptides and fragments thereof.

Native crystals of the present invention can be grown by dissolving a substantially pure CAR polypeptide or a fragment thereof, and optionally a

-83-

ligand, in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

In one embodiment of the invention, native crystals are grown by vapor diffusion (See e.g., McPherson, 1982; McPherson, 1990). In this method, the polypeptide/precipitant solution is allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration optimal for producing crystals. Generally, less than about 25 µL of CAR polypeptide solution is mixed with an equal volume of reservoir solution, giving a precipitant concentration about half that required for crystallization. This solution is suspended as a droplet underneath a coverslip, which is sealed onto the top of the reservoir. The sealed container is allowed to stand until crystals grow. Crystals generally form within two to six weeks, and are suitable for data collection within approximately seven to ten weeks. Of course, those of skill in the art will recognize that the above-described crystallization procedures and conditions can be varied.

VIII. Solving a Crystal Structure of the Present Invention

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Crystal structures of the present invention can be solved using a variety of techniques including, but not limited to isomorphous replacement, anomalous scattering, or molecular replacement methods. Computer software packages can also be used to solve a crystal structure of the present invention. Applicable software packages include, but are not limited to X-PLOR™ program (Brünger, 1992; available from Accelrys Inc, San Diego, California, United States of America), Xtal View (McRee, 1992; available from the San Diego Supercomputer Center, San Diego, California, United States of America); SHELXS 97 (Sheldrick, 1990; available from the Institute of Inorganic Chemistry, Georg-August-Universität, Göttingen, Germany); HEAVY (Terwilliger, Los Alamos National Laboratory) and SHAKE-AND-BAKE (Hauptman, 1997; Weeks et al., 1993; available from the Hauptman-

Woodward Medical Research Institute, Buffalo, New York, United States of America). See also, Ducruix & Geige, 1992, and references cited therein.

IX. The Overall Structure of CARα in Complex With a Ligand

The structure of the LBD of CAR bound with Compound 1 has been determined to 2.15Å. The statistics of the data and the refined structure are summarized in Table 1.

<u>Table 1</u>
Statistics of Crystallographic Data and Structure

Crystals	CAR/ with Compound 1
Space group	P2 ₁ 2 ₁ 2 ₁
Resolution (Å)	40.0- 2.15
Unique reflections	69,338
Completeness (%)	99.6
I/g(last shell)	21.7 (3.1)
R _{sym} ^a (%)	9.1
Refinement statistics	
R factor ^b (%)	21.5
R free (%)	25.1
R.M.S.D.	
bond lengths (Å)	0.007
R.M.S.D.	
bond angles(degrees)	1.308
Total non-hydrogen atoms	
	8601

R.M.S.D. is the root mean square deviation from ideal geometry. ${}^{a}R_{sym} = \sum |lavg - li| / \sum li$

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 $^{^{}b}R_{factor} = \sum |F_{P} - F_{Pcalc}| / \sum F_{p}$, where F_{p} and F_{pcalc} are observed and calculated structure factors, R_{free} is calculated from a randomly chosen 10% of reflections that were never used in refinement and R_{factor} is calculated for the remaining 90% of reflections.

In its complex with Compound 1, an inverse agonist, the CAR LBD has a structure with approximately 11 alpha helices and a beta-sheet with 3 strands, as shown in Figure 1. The CAR LBD amino acid sequence is more similar to PXR and VDR than to any other NR LBD sequence, with 50% identity to PXR and 40% identity to VDR in a core region corresponding to VDR residues 126-142, 227-289, 293-300, 302-404 and 416-421. Slightly lower percent identities are obtained by considering the entire LBD sequences; however, these percent identities are complicated by the presence of additional amino acids inserted between Helix-1 and Helix-3 in PXR.

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Figure 2 gives an alignment of the human, mouse, and rat CAR sequences with the human PXR and CAR sequences, with annotation and shading to indicate structural features identified from the X-ray structures. The AF2 helix that is normally present in NR LBDs was absent in this structure, but another helix, designated here as "helix-X", was present. Helix-X includes Leu336, Ser337, Ala338, and Met339, which lie between helix-10 and the residues that normally form the AF2 helix. The hydrogen bonding pattern in helix-X is closer to that of a 3-10 helix rather than an ideal alpha helix. The absence of the AF2 helix was initially very surprising, since the amino acid sequence at the C-terminal end of CAR is very similar to the corresponding segments in VDR and PXR (Figure 2), where the AF2 helix has been seen in all available X-ray structures. Normally, activation of gene transcription depends on the binding of a coactivator, such as CREB binding protein (CBP) or steroid receptor coactivator-1 (SRC-1), and this in turn normally requires the presence of the AF2 helix in its active position. Thus, one would expect the AF2 helix to be present and in the active position in the unliganded, constitutively active form of CAR.

An inverse agonist such as Compound 1 or an antagonist could reduce gene transcription by shifting the AF2 helix into an alternative position, as has been observed with estrogen receptor (ER) bound to antagonists such as tamoxifen and raloxifene (Shiau *et al.*, 1998). Alternatively, an inverse agonist

or antagonist could act by unwinding the AF2 helix without necessarily moving it from its active position. Further analysis of the CAR X-ray structure suggests that helix-X interferes with the formation of the AF2 helix. Also, side-chains from Met339 and Met340, in and adjacent to helix-X, make extensive interactions with Compound 1. This suggests that Compound 1 induces the formation of helix-X, which in turn unwinds the AF2 helix, thereby preventing coactivator binding and shutting down gene transcription.

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More generally, the analysis of the X-ray structure suggests that CAR exists in equilibrium with at least two major conformations. One conformation is an "activated conformation", not yet observed by X-ray crystallography. where the AF2 helix is properly formed and resides in its active position. The second major conformation is an inactivated conformation, exemplified by the complex of CAR with Compound 1, where helix-X is present and the AF2 helix is absent. While the inventors do not wish to be bound by any particular hypothesized mechanism of action, it appears that, in the absence of ligand, CAR exists predominantly in the activated conformation. Agonist and "superagonist" compounds would tend to shift the equilibrium even farther towards this activated form, effectively increasing the fraction of the CAR receptor in the activated state to a level higher than that observed in the absence of ligand. Inverse agonists, such as Compound 1, would act by shifting the equilibrium towards the inactivated conformation, effectively decreasing the fraction of the CAR receptor in the activated state.

The structure of CAR revealed a number of other major structural differences when compared with the structures of PXR and VDR. The CAR X-ray structure allowed an accurate alignment of helix-1, confirming that PXR and VDR have 45 and 51 additional residues, respectively, in the region between helix-1 and helix-3. The conformation of this insert is unknown in VDR, as the available X-ray structures were determined with a construct where this insert was deleted. The full insert was present in the construct used for the PXR X-ray structure, and most of the insert was visible in the electron density. Surprisingly, in PXR, a segment from this insert acts to displace helix-6 from its usual position where it covers the ligand-binding

pocket. This segment adopts an extended conformation that occupies less volume than helix-6, effectively opening up additional volume for the ligand in the PXR ligand-binding pocket. While the inventors do not wish to be bound by any particular hypothesized mechanism of action, based on the PXR X-ray structure and the similarity of the CAR amino acid sequence to PXR, one might expect that helix-6 would be absent or displaced away from the ligandbinding pocket, and that the ligand-binding pocket would be similarly voluminous. However, the X-ray structure of CAR reveals that helix-6 is present in CAR, and located in a position similar to that in VDR where it serves as one wall for the ligand-binding pocket. This reduces the volume available to the ligand in the ligand-binding pocket, and changes the shape of the pocket substantially. The pocket volume was calculated with the GRASP program using the atomic radii of Bondi, 1964, using a procedure where the MVP program is used to close channels to the external solvent. With this procedure, the CAR pocket has a volume of 824 Å³, similar to that of VDR. which has a volume of 871 Å³ when bound to Vitamin D, but much smaller than PXR, which has a volume of 1150-1544 Å³, depending on the ligand complexed to the protein.

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The structure of the LBD of CAR comprises 11 main alpha helices, a beta sheet with 4 strands, and additional irregular structure and shorter helices. The key features are shown in Figure 1. Helices 3, 5, 6, 7, and 10 and beta strands 2, 3, and 4 enclose the ligand-binding pocket, like a three-layer sandwich (Figure 6). Helix 6, which is absent or displaced in PXR, is intact in CAR, and located in a position similar to that in VDR where it serves as part of the wall of the ligand-binding site. The structure-based sequence alignment of Figure 2 shows the secondary structures of CAR, PXR, and VDR. The presence of helix 6 in CAR reduces the size of the ligand-binding site. The limited binding pocket gives more selectivity in ligand-binding in CAR than in PXR. Binding of the antagonist in CAR causes the AF2 helix to unwind. Instead, a short sequence of amino acids located between helix 10 and the AF2 helix (Leu336, Ser337, Ala338, Met339) form a short 3-10 helix. The side chains of Leu336 and Met339, from the 3-10 helix, and Met340 form

a wall that nicely fits the side of the phenyl ring of the ligand (Figure 1 & 3). This 3-10 helix is referred to as helix X. Steric hindrance from helix X appears to contribute to the unwinding of AF2 helix

The ligand-binding site can be divided into two chambers (Figure 5). One chamber contains the phenylethyl and benzimidazole-6-carboxamide fragments of the ligand. It is completely shielded from solvent. The other chamber contains the benzhydryl fragment of the ligand. This chamber is exposed to the solvent. The amino linker of the ligand is near the interface of the two chambers.

Figure 3 and 4 shows that the ligand fits nicely into the hydrophobic pocket of the LBD site formed mostly by aromatic or hydrophobic residues. They are Phe132, Phe161, Ile164, Asn165, Thr166, Met168, Val169, Ala198, Val199, Cys202, His203, Leu206, Phe217, Tyr224, Thr225, Ile226, Glu227, Asp228, Gly229, Ala230, Phe234, Phe238, Leu239, Leu242, Phe243, His246, Tyr326, Ile330, Leu336, Ser337, Met339, and Met340.

As shown in Figure 3 and 4, there are four hydrogen bonds between the ligand and LBD. The benzimidazol-6-carboxamide forms hydrogen bonds with the carbonyl oxygen of Thr225 and Gly229 amide, respectively. The unsubstituted nitrogen on the benzimidazole forms a hydrogen bond with the hydroxyl group of Tyr326. The amino group linked to the benzhydryl forms a hydrogen bond with the carboxyl oxygen of Asn165. The later two hydrogen bonds are located near the intersection of the two chambers.

X. Rational Drug Design

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X.A. Generally

Modulators to polypeptides of the invention and other structurally related molecules, and complexes containing the same, can be identified and developed as set forth below and otherwise using techniques and methods known to those of skill in the art.

The present invention contemplates making any molecule that is shown to modulate the activity of a polypeptide of the invention.

-89-

In another embodiment, inhibitors, modulators of the subject polypeptides, or biological complexes containing them, can be used in the manufacture of a medicament for any number of uses, including, for example, treating any disease or other treatable condition of a patient (including humans and animals), and particularly a disease caused by aberrant CAR regulation or activity.

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A number of techniques can be used to screen, identify, select, and design chemical entities capable of associating with polypeptides of the invention, structurally homologous molecules, and other molecules. Knowledge of the structure for a polypeptide of the invention, determined in accordance with the methods described herein, permits the design and/or identification of molecules and/or other modulators which have a shape complementary to the conformation of a polypeptide of the invention, or more particularly, a druggable region thereof. It is understood that such techniques and methods can use, in addition to the exact structural coordinates and other information for a polypeptide of the invention, structural equivalents thereof described above (including, for example, those structural coordinates that are derived from the structural coordinates of amino acids contained in a druggable region as described above).

The term "chemical entity", as used herein, refers to chemical compounds, complexes of two or more chemical compounds, and fragments of such compounds or complexes. In certain instances, it is desirable to use chemical entities exhibiting a wide range of structural and functional diversity, such as compounds exhibiting different shapes (*i.e.*, flat aromatic rings(s), puckered aliphatic rings(s), straight and branched chain aliphatics with single, double, or triple bonds) and diverse functional groups (*i.e.*, carboxylic acids, esters, ethers, amines, aldehydes, ketones, and various heterocyclic rings).

In one aspect, the method of drug design generally includes computationally evaluating the potential of a selected chemical entity to associate with any of the molecules or complexes of the present invention (or portions thereof). For example, this method can include the steps of (a) employing computational means to perform a fitting operation between the

selected chemical entity and a druggable region of the molecule or complex; and (b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the druggable region.

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A chemical entity can be examined either through visual inspection or through the use of computer modeling using a docking program such as GRAM, DOCK, or AUTODOCK (Dunbrack et al., 1997). This procedure can include computer fitting of chemical entities to a target to ascertain how well the shape and the chemical structure of each chemical entity will complement or interfere with the structure of the subject polypeptide (Bugg et al., 1993; West et al., 1995). Computer programs can also be employed to estimate the attraction, repulsion, and steric hindrance of the chemical entity to a druggable region, for example. Generally, the tighter the fit (i.e., the lower the steric hindrance, and/or the greater the attractive force) the more potent the chemical entity will be because these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a chemical entity the more likely that the chemical entity will not interfere with related proteins, which can minimize potential side-effects due to unwanted interactions.

A variety of computational methods for molecular design, in which the steric and electronic properties of druggable regions are used to guide the design of chemical entities, are known. See e.g., Cohen et al., 1990; Kuntz et al., 1982; DesJarlais, 1988; Bartlett et al., 1989; Goodford et al., 1985; DesJarlais et al., 1986. Directed methods generally fall into two categories: (1) design by analogy in which 3-D structures of known chemical entities (such as from a crystallographic database) are docked to the druggable region and scored for goodness-of-fit; and (2) de novo design, in which the chemical entity is constructed piece-wise in the druggable region. The chemical entity can be screened as part of a library or a database of molecules. Databases which can be used include ACD (MDL Systems Inc., San Leandro, California, United States of America), NCI (National Cancer Institute, Bethesda, Maryland, United States of America), CCDC (Cambridge Crystallographic Data Center, Cambridge, England, United Kingdom), CAST

-91-

(Chemical Abstract Service), Derwent (Derwent Information Limited, London, England, United Kingdom), Maybridge (Maybridge Chemical Company Ltd., Cornwall, England, United Kingdom), Aldrich (Aldrich Chemical Company, St. Louis, Missouri, United States of America), DOCK (University of California in San Francisco, San Francisco, California, United States of America), and the Directory of Natural Products (Chapman & Hall). Computer programs such as CONCORD (Tripos Inc., St. Louis, Missouri, United States of America) or DB-Converter (Molecular Simulations Limited, Cambridge, England, United Kingdom) can be used to convert a data set represented in two dimensions to one represented in three dimensions.

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Chemical entities can be tested for their capacity to fit spatially with a druggable region or other portion of a target protein. As used herein, the term "fits spatially" means that the three-dimensional structure of the chemical entity is accommodated geometrically by a druggable region. A favorable geometric fit occurs when the surface area of the chemical entity is in close proximity with the surface area of the druggable region without forming unfavorable interactions. A favorable complementary interaction occurs where the chemical entity interacts by hydrophobic, aromatic, ionic, dipolar, or hydrogen donating and accepting forces. Unfavorable interactions can be steric hindrance between atoms in the chemical entity and atoms in the druggable region.

If a model of the present invention is a computer model, the chemical entities can be positioned in a druggable region through computational docking. If, on the other hand, the model of the present invention is a structural model, the chemical entities can be positioned in the druggable region by, for example, manual docking. As used herein the term "docking" refers to a process of placing a chemical entity in close proximity with a druggable region, or a process of finding low energy conformations of a chemical entity/druggable region complex.

In an illustrative embodiment, the design of potential modulator begins from the general perspective of shape complimentary for the druggable region of a polypeptide of the invention, and a search algorithm is employed which is

capable of scanning a database of small molecules of known three-dimensional structure for chemical entities which fit geometrically with the target druggable region. Most algorithms of this type provide a method for finding a wide assortment of chemical entities that are complementary to the shape of a druggable region of the subject polypeptide. Each of a set of chemical entities from a particular data-base, such as the Cambridge Crystallographic Data Bank (CCDB) (Allen et al., 1973), is individually docked to the druggable region of a polypeptide of the invention in a number of geometrically permissible orientations with use of a docking algorithm. In certain embodiments, a set of computer algorithms called DOCK, can be used to characterize the shape of invaginations and grooves that form the active sites and recognition surfaces of the druggable region (Kuntz et al., 1982). The program can also search a database of small molecules for templates whose shapes are complementary to particular binding sites of a polypeptide of the invention (DesJarlais et al., 1988).

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The orientations are evaluated for goodness-of-fit and the best are kept for further examination using molecular mechanics programs, such as AMBER or CHARMM. Such algorithms have previously proven successful in finding a variety of chemical entities that are complementary in shape to a druggable region.

Goodford et al., 1985 and Boobbyer et al., 1989 have produced a computer program (GRID) that seeks to determine regions of high affinity for different chemical groups (termed probes) of the druggable region. GRID hence provides a tool for suggesting modifications to known chemical entities that might enhance binding. It can be anticipated that some of the sites discerned by GRID as regions of high affinity correspond to "pharmacophoric patterns" determined inferentially from a series of known ligands. As used herein, a "pharmacophoric pattern" is a geometric arrangement of features of chemical entities that is believed to be important for binding. Attempts have been made to use pharmacophoric patterns as a search screen for novel ligands (Jakes et al., 1987; Brint & Willett, 1987; Jakes et al., 1986).

Yet a further embodiment of the present invention utilizes a computer algorithm such as CLIX which searches such databases as CCDB for chemical entities which can be oriented with the druggable region in a way that is both sterically acceptable and has a high likelihood of achieving favorable chemical interactions between the chemical entity and the surrounding amino acid residues. The method is based on characterizing the region in terms of an ensemble of favorable binding positions for different chemical groups and then searching for orientations of the chemical entities that cause maximum spatial coincidence of individual candidate chemical groups with members of the ensemble. The algorithmic details of CLIX are described in Lawrence et al., 1992.

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In this way, the efficiency with which a chemical entity can bind to or interfere with a druggable region can be tested and optimized by computational evaluation. For example, for a favorable association with a druggable region, a chemical entity must preferably demonstrate a relatively small difference in energy between its bound and fine states (*i.e.*, a small deformation energy of binding). Thus, certain, more desirable chemical entities will be designed with a deformation energy of binding of not greater than about 10 kcal/mole, and more preferably, not greater than 7 kcal/mole. Chemical entities can interact with a druggable region in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the chemical entity binds to the target.

In this way, the present invention provides computer-assisted methods for identifying or designing a potential modulator of the activity of a polypeptide of the invention including: supplying a computer modeling application with a set of structure coordinates of a molecule or complex, the molecule or complex including at least a portion of a druggable region from a polypeptide of the invention; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to the molecule or complex, wherein

-94-

binding to the molecule or complex is indicative of potential modulation of the activity of a polypeptide of the invention.

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In another aspect, the present invention provides a computer-assisted method for identifying or designing a potential modulator to a polypeptide of the invention, supplying a computer modeling application with a set of structure coordinates of a molecule or complex, the molecule or complex including at least a portion of a druggable region of a polypeptide of the invention; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding interactions between the chemical entity and active site of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity, and determining whether the modified chemical entity is expected to bind to the molecule or complex, wherein binding to the molecule or complex is indicative of potential modulation of the polypeptide of the invention.

In one embodiment, a potential modulator can be obtained by screening a peptide library (Scott & Smith, 1990; Cwirla et al., 1990; Devlin et al., 1990). A potential modulator selected in this manner could then be systematically modified by computer modeling programs until one or more promising potential drugs are identified. Such analysis has been shown to be effective in the development of HIV protease inhibitors (Lam et al., 1994; Wlodawer et al., 1993; Appelt, 1993; Erickson, 1993). Alternatively a potential modulator can be selected from a library of chemicals such as those that can be licensed from third parties, such as chemical and pharmaceutical companies. A third alternative is to synthesize the potential modulator de novo.

For example, in certain embodiments, the present invention provides a method for making a potential modulator for a polypeptide of the invention, the method including synthesizing a chemical entity or a molecule containing the chemical entity to yield a potential modulator of a polypeptide of the invention, the chemical entity having been identified during a computer-assisted process including supplying a computer modeling application with a set of structure

-95-

coordinates of a molecule or complex, the molecule or complex including at least one druggable region from a polypeptide of the invention; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to the molecule or complex at the active site, wherein binding to the molecule or complex is indicative of potential modulation. This method can further include the steps of evaluating the potential binding interactions between the chemical entity and the active site of the molecule or molecular complex and structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity, which steps can be repeated one or more times.

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Once a potential modulator is identified, it can then be tested in any standard assay for the macromolecule depending of course on the macromolecule, including in high throughput assays. Further refinements to the structure of the modulator will generally be necessary and can be made by the successive iterations of any and/or all of the steps provided by the particular screening assay, in particular further structural analysis by *i.e.*, 15N NMR relaxation rate determinations or X-ray crystallography with the modulator bound to the subject polypeptide. These studies can be performed in conjunction with biochemical assays.

Once identified, a potential modulator can be used as a model structure, and analogs to the compound can be obtained. The analogs are then screened for their ability to bind the subject polypeptide. An analog of the potential modulator might be chosen as a modulator when it binds to the subject polypeptide with a higher binding affinity than the predecessor modulator.

In a related approach, iterative drug design is used to identify modulators of a target protein. Iterative drug design is a method for optimizing associations between a protein and a modulator by determining and evaluating the three dimensional structures of successive sets of protein/modulator complexes. In iterative drug design, crystals of a series of protein/modulator complexes are obtained and then the three-dimensional

-96-

structures of each complex is solved. Such an approach provides insight into the association between the proteins and modulators of each complex. For example, this approach can be accomplished by selecting modulators with inhibitory activity, obtaining crystals of this new protein/modulator complex, solving the three dimensional structure of the complex, and comparing the associations between the new protein/modulator complex and previously solved protein/modulator complexes. By observing how changes in the modulator affected the protein/modulator associations, these associations can be optimized.

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In addition to designing and/or identifying a chemical entity to associate with a druggable region, as described above, the same techniques and methods can be used to design and/or identify chemical entities that either associate, or do not associate, with affinity regions, selectivity regions or undesired regions of protein targets. By such methods, selectivity for one or a few targets, or alternatively for multiple targets, from the same species or from multiple species, can be achieved.

For example, a chemical entity can be designed and/or identified for which the binding energy for one druggable region, *i.e.*, an affinity region or selectivity region, is more favorable than that for another region, *i.e.*, an undesired region, by about 20%, 30%, 50% to about 60% or more. It can be the case that the difference is observed between (a) more than two regions, (b) between different regions (selectivity, affinity or undesirable) from the same target, (c) between regions of different targets, (d) between regions of homologs from different species, or (e) between other combinations. Alternatively, the comparison can be made by reference to the K_d , usually the apparent K_d , of said chemical entity with the two or more regions in question.

In another aspect, prospective modulators are screened for binding to two nearby druggable regions on a target protein. For example, a modulator that binds a first region of a target polypeptide does not bind a second nearby region. Binding to the second region can be determined by monitoring changes in a different set of amide chemical shifts in either the original screen or a second screen conducted in the presence of a modulator (or potential

modulator) for the first region. From an analysis of the chemical shift changes, the approximate location of a potential modulator for the second region is identified. Optimization of the second modulator for binding to the region is then carried out by screening structurally related compounds (*i.e.*, analogs as described above).

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When modulators for the first region and the second region are identified, their location and orientation in the ternary complex can be determined experimentally. On the basis of this structural information, a linked compound, i.e., a consolidated modulator, is synthesized in which the modulator for the first region and the modulator for the second region are linked. In certain embodiments, the two modulators are covalently linked to form a consolidated modulator. This consolidated modulator can be tested to determine if it has a higher binding affinity for the target than either of the two individual modulators. A consolidated modulator is selected as a modulator when it has a higher binding affinity for the target than either of the two modulators. Larger consolidated modulators can be constructed in an analogous manner, i.e., linking three modulators which bind to three nearby regions on the target to form a multilinked consolidated modulator that has an even higher affinity for the target than the linked modulator. In this example, it is assumed that is desirable to have the modulator bind to all the druggable regions. However, it can be the case that binding to certain of the druggable regions is not desirable, so that the same techniques can be used to identify modulators and consolidated modulators that show increased specificity based on binding to at least one but not all druggable regions of a target.

The present invention provides a number of methods that use drug design as described above. For example, in one aspect, the present invention contemplates a method for designing a candidate compound for screening for inhibitors of a polypeptide of the invention, the method comprising: (a) determining the three dimensional structure of a crystallized polypeptide of the invention or a fragment thereof; and (b) designing a candidate inhibitor based on the three dimensional structure of the crystallized polypeptide or fragment.

In another aspect, the present invention provides a method for identifying a potential inhibitor of a polypeptide of the invention, the method comprising: (a) providing the three-dimensional coordinates of a polypeptide of the invention or a fragment thereof; (b) identifying a druggable region of the polypeptide or fragment; and (c) selecting from a database at least one compound that comprises three dimensional coordinates which indicate that the compound can bind the druggable region; (d) wherein the selected compound is a potential inhibitor of a polypeptide of the invention.

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In another aspect, the present invention contemplates a method for identifying a potential modulator of a molecule comprising a druggable region similar to that of SEQ ID NO: 2 or SEQ ID NO: 4, the method comprising: (a) using the atomic coordinates of amino acid residues from SEQ ID NO: 2 or SEQ ID NO: 4, or a fragment thereof, ± a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5 Å, to generate a three-dimensional structure of a molecule comprising a druggable region that is a portion of SEQ ID NO: 2 or SEQ ID NO: 4; (b) employing the three dimensional structure to design or select the potential modulator; (c) synthesizing the modulator; and (d) contacting the modulator with the molecule to determine the ability of the modulator to interact with the molecule.

In another aspect, the present invention contemplates an apparatus for determining whether a compound is a potential inhibitor of a polypeptide having SEQ ID NO: 2 or SEQ ID NO: 4, the apparatus comprising: (a) a memory that comprises: (i) the three dimensional coordinates and identities of the atoms of a polypeptide of the invention or a fragment thereof that form a druggable site; and (ii) executable instructions; and (b) a processor that is capable of executing instructions to: (i) receive three-dimensional structural information for a candidate compound; (ii) determine if the three-dimensional structure of the candidate compound is complementary to the structure of the interior of the druggable site; and (iii) output the results of the determination.

In another aspect, the present invention contemplates a method for designing a potential compound for the prevention or treatment of a disease

-99-

or disorder, the method comprising: (a) providing the three dimensional structure of a crystallized polypeptide of the invention, or a fragment thereof; (b) synthesizing a potential compound for the prevention or treatment of a disease or disorder based on the three dimensional structure of the crystallized polypeptide or fragment; (c) contacting a polypeptide of the present invention or a PDE with the potential compound; and (d) assaying the activity of a polypeptide of the present invention, wherein a change in the activity of the polypeptide indicates that the compound can be useful for prevention or treatment of a disease or disorder.

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In another aspect, the present invention contemplates a method for designing a potential compound for the prevention or treatment of a disease or disorder, the method comprising: (a) providing structural information of a druggable region derived from NMR spectroscopy of a polypeptide of the invention, or a fragment thereof; (b) synthesizing a potential compound for the prevention or treatment of a disease or disorder based on the structural information; (c) contacting a polypeptide of the present invention or a PDE with the potential compound; and (d) assaying the activity of a polypeptide of the present invention, wherein a change in the activity of the polypeptide indicates that the compound can be useful for prevention or treatment of a disease or disorder.

X.B. Methods of Designing CAR LBD Ligand Compounds

As discussed above, the analysis of the CAR X-ray structure suggests that CAR can adopt at least two major conformations. One major conformation corresponds to the activated state of CAR, where helix-X is absent, and where the AF2 helix is properly formed and resides in its active position. The second major conformation corresponds to the inactivated conformation, exemplified by the complex of CAR with Compound 1, where helix-X is present and where the AF2 helix is absent. In both conformations, the ligand-binding pocket is capped by the C-terminal tail, residues 340-348. These residues adopt different conformations in the activated and inactivated states of CAR, effectively covering the pocket with a cap that can assume at

-100-

least two alternative shapes. Some CAR ligands might bind preferentially to the activated conformation of CAR, whereas some other CAR ligands might bind preferentially to the inactivated conformation of CAR. There might also be some ligands that bind equally well to either conformation of CAR. When a ligand binds preferentially to a particular conformational state, it will lower the energy of that state, thereby shifting the equilibrium towards that state, and increasing the fraction of the CAR receptor that exists in that state. This thermodynamic principle can be used together with the three dimensional structure of CAR to design chemical compounds that bind to specific conformational states of CAR, thereby increasing or decreasing the level of transcription in genes regulated by CAR.

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The present X-ray structure of CAR bound to Compound 1 provides an accurate three-dimensional structure of the ligand-binding pocket in the inactivated conformational state of CAR. Novel ligands can be designed to fit this specific pocket using a variety of computational methods, discussed below. Alternatively, known ligands can be docked into the ligand-binding pocket, using a variety of docking programs and algorithms. These docked structures can be examined graphically to suggest chemical modifications that would improve their fit to the pocket, or their binding to the receptor. Alternatively, known ligands can be complexed with the CAR protein and crystallized using the methods of this invention, allowing the structure of the complex to be determined by X-ray crystallography. The three dimensional structures can be examined graphically to suggest chemical modifications that would improve their fit to the pocket, or their binding to the receptor.

The present X-ray structure of CAR can also be used as a template to build a three-dimensional model of the structure of the activated form of CAR. For example, residues 107 to 332, corresponding to helix-1 through most of helix-10, are taken to have exactly the same coordinates as in the template CAR structure. The AF2 helix, CAR residues 341-348, is then built using the structure of VDR as the template. The VDR template structure is superimposed onto the CAR structure using standard methods as disclosed herein and as would be apparent to one of ordinary skill in the art after a

-101-

review of the present disclosure. The AF2 helix from VDR, residues 416-423, is then removed from the VDR template and transplanted into the model for CAR, without any adjustment of its coordinates. Five of the residues in the VDR AF2 helix have amino acid types different from the corresponding residues in the CAR AF2 helix. These residues are VDR Val418, Leu419, Val421, Phe422, and Gly423, which correspond to CAR Leu343, Gln344, Ile346, Cys347, and Ser348, respectively. These five residues are computationally "mutated" in the model, to obtain the covalent structure corresponding to the desired amino acids in CAR. The C-terminal Ser348 is further modified to obtain a free carboxylate as normally occurs at the C-terminal end of a protein chain.

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These computational mutations can be carried out using amino acid replacement and builder functionality in molecular graphics programs such as Insight-II, available from Accelrys, or using non-graphical molecular mechanics software such as MVP. The side-chain conformations are then adjusted using computer graphics, such as Insight-II, or other energy-based procedures, such as in MVP, to obtain a reasonable overall fit. It is more difficult to obtain a reasonable conformation for the eight residues in the AF2 linker. CAR residues 333-340. The VDR linker, residues 407-415, cannot be used as the template for the CAR linker because it has nine residues, and because its N-terminal end-point is different from that required in CAR. Likewise, the PXR linker, residues 418-422, is too short to serve as a template for the CAR linker. For structure-based drug design, a conservative approach is to omit the linker residues rather than to model the linker incorrectly. Consequently, in one embodiment the linker, residues 333-340, is omitted from the activated CAR model. This model for the activated state of CAR then provides a binding site for the ligand design processes described elsewhere herein. Specifically, various computer software programs can be used to design novel ligands that would fit the specific pocket in the model for the activated form of CAR. Docking calculations can be used to predict how known CAR activators will bind to the activated form of CAR or to identify other available compounds that might bind. These predicted complex

-102-

structures can then be examined by computer graphics to suggest specific chemical modifications that would enhance the binding to the activated state of CAR.

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To be useful as a therapeutic agent, a chemical compound that acts through CAR must induce the appropriate level of CAR activity in relevant tissues. In principle, this can be achieved by adjusting the CAR conformational equilibrium so that appropriate fractions of the CAR protein exist in the activated and inactivated states. This in turn can be achieved with ligands that bind almost exclusively to one or the other of the two major conformational states. The design of ligands that are selective for a specific conformational state is facilitated by consideration of how these ligands might bind to each of the two conformational states. Binding modes can be obtained using docking calculations, and then examined graphically to suggest chemical modifications that would make binding to a particular conformational state either more favorable or less favorable. Iterative application of these techniques can yield ligands with the desired level of selectivity for the particular conformational state of CAR, thereby achieving the desired level of CAR activity. Ligands that can bind to both conformational states of the CAR protein can also be designed. This is also facilitated by consideration of how the ligands might bind to each of the two conformational states, using the same approach as discussed above, but this time seeking chemical structures and chemical modifications that would permit binding to both conformational states.

The methods of this invention can also be used to suggest possible chemical modifications of a compound that might reduce or minimize its effect on CAR. This approach can be useful in drug discovery projects aiming to find compounds that modulate the activity of some other target molecule, where modulation of CAR activity is an undesirable side effect. This approach is useful in engineering CAR activity out of other, non-drug molecules. Humans and other animals are exposed to a wide range of different chemical compounds, some of which might act on CAR in an undesirable manner. Such a compound could be complexed with CAR and crystallized using the

-103-

methods of the present invention. The structure could then be determined by X-ray crystallography. Alternatively, the structure of the complex could be predicted computationally using molecular docking software. In this case, compounds that tend to activate CAR would be docked into a model or structure of the activated form of CAR, whereas compounds that tend to reduce the activity of CAR would be docked into a model or structure of an inactivated form of CAR, such as its complex with Compound 1 presented here.

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Whether the structure is obtained by X-ray crystallography or computational methods, the structure would be examined by computer graphics to suggest chemical modifications that would minimize the tendency to bind to CAR. For example, substituents could be introduced onto the compound that would project into volume occupied by the CAR protein. Alternatively, a region of the molecule that binds to a lipophilic region of the CAR binding site could be modified to make it more polar, thus reducing its tendency to bind to CAR. Alternatively, a polar group of the compound that makes a hydrogen bonding interaction with CAR could be identified and modified to an alternative group that fails to make the hydrogen bond. Appropriate chemical modifications can be chosen such that the desirable properties and behavior of the compound would be retained.

The design of candidate substances, also referred to as "compounds" or "candidate compounds", that bind to or modulate nuclear receptor (NR) LBD (for example, CAR LBD) -mediated activity according to the present invention generally involves consideration of two factors. First, the compound must be capable of chemically and structurally associating with a NR LBD. Non-covalent molecular interactions important in the association of a NR LBD with its substrate include hydrogen bonding, van der Waals interactions, and hydrophobic interactions. The interaction between an atom of an LBD amino acid and an atom of an LBD ligand can be made by any force or attraction described in nature. Usually the interaction between the atom of the amino acid and the ligand will be the result of a hydrogen bonding interaction, charge interaction, hydrophobic interaction, van der Waals interaction, or dipole

-104-

interaction. In the case of the hydrophobic interaction, it is recognized that this is not a per se interaction between the amino acid and ligand, but rather the usual result, in part, of the repulsion of water or other hydrophilic groups from a hydrophobic surface. Reducing or enhancing the interaction of the LBD and a ligand can be measured by calculating or testing binding energies, either computationally or using thermodynamic or kinetic methods known in the art.

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Second, the compound must be able to assume a conformation that allows it to associate with a NR LBD. Although certain portions of the compound will not directly participate in this association with a NR LBD, those portions can still influence the overall conformation of the molecule. This influence on conformation, in turn, can have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., the ligand-binding pocket or an accessory binding site of a NR LBD, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with a NR LBD.

Chemical modifications can enhance or reduce interactions of an atom of a LBD amino acid and an atom of an LBD ligand. Steric hindrance can be a common approach for changing the interaction of a LBD binding pocket with an activation domain. Chemical modifications are introduced in one embodiment at C-H, C-, and C-OH positions in a ligand, where the carbon is part of the ligand structure that remains the same after modification is complete. In the case of C-H, C could have 1, 2, or 3 hydrogens, but usually only one hydrogen will be replaced. The H or OH can be removed after modification is complete and replaced with a desired chemical moiety.

The potential binding effect of a chemical compound on a NR LBD can be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques that employ the coordinates of a crystalline NR LBD, for example a CAR LBD polypeptide of the present invention. If the theoretical structure of the given compound suggests insufficient interaction and

-105-

association between it and a NR LBD, synthesis and testing of the compound is obviated. However, if computer modeling indicates a strong interaction, the molecule can then be synthesized and tested for its ability to bind and modulate the activity of a NR LBD. In this manner, synthesis of unproductive or inactive compounds can be avoided.

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A binding compound of a NR LBD polypeptide (in one embodiment a CAR LBD) can be computationally evaluated and designed via a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with an individual binding site or other area of a crystalline CAR LBD polypeptide of the present invention and to interact with the amino acids disposed in the binding sites.

Interacting amino acids forming contacts with a ligand and the atoms of the interacting amino acids are usually 2 to 4 angstroms away from the center of the atoms of the ligand. Generally these distances are determined by computer as discussed herein and in McRee, 1993. However distances can be determined manually once the three dimensional model is made. More commonly, the atoms of the ligand and the atoms of interacting amino acids are 3 to 4 angstroms apart. A ligand can also interact with distant amino acids, after chemical modification of the ligand to create a new ligand. Distant amino acids are generally not in contact with the ligand before chemical modification. A chemical modification can change the structure of the ligand to make a new ligand that interacts with a distant amino acid usually at least 4.5 angstroms away from the ligand. Distant amino acids rarely line the surface of the binding cavity for the ligand, as they are too far away from the ligand to be part of a pocket or surface of the binding cavity.

A compound designed or selected as binding to an NR polypeptide (in one embodiment a CAR LBD polypeptide) can be further computationally optimized so that in its bound state it would lack repulsive electrostatic interaction with the target polypeptide. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole, and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the ligand and the polypeptide when the ligand is bound

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to an NR LBD make a neutral or favorable contribution to the enthalpy of binding.

One of several methods can be used to screen chemical entities or fragments for their ability to associate with a NR LBD and, more particularly, with the individual binding sites of a NR LBD, such as a ligand-binding pocket or an accessory binding site. This process can begin by visual inspection of, for example, a ligand-binding pocket on a computer screen based on the CAR LBD atomic coordinates disclosed in Tables 2-3. Selected fragments or chemical entities can then be positioned in a variety of orientations, or docked, within an individual binding site of a CAR LBD as defined herein above. Docking can be accomplished using software programs such as those available under the trade names QUANTA™ (available from Accelrys Inc, San Diego, California, United States of America) and SYBYL™ (available from Tripos, Inc., St. Louis, Missouri, United States of America), followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARM (Brooks *et al.*, 1993) and AMBER 5 (Case *et al.*, 1997; Pearlman *et al.*, 1995).

Specialized computer programs can also assist in the process of selecting fragments or chemical entities. These include:

- 1. GRID™ program, version 17 (Goodford, 1985), which is available from Molecular Discovery Ltd. of Oxford, United Kingdom;
- 2. MCSS™ program (Miranker & Karplus, 1991), which is available from Accelrys Inc, San Diego, California, United States of America;
- 3. AUTODOCK™ 3.0 program (Goodsell & Olsen, 1990), which is available from the Scripps Research Institute, La Jolla, California, United States of America;
- 4. DOCK™ 4.0 program (Kuntz et al., 1992), which is available from the University of California, San Francisco, California, United States of America:
- 5. FLEX-X™ program (See Rarey et al., 1996), which is available from Tripos, Inc., St. Louis, Missouri, United States of America;
 - 6. MVP program (Lambert, 1997); and

-107-

7. LUDI™ program (Bohm, 1992), which is available from Accelrys Inc, San Diego, California, United States of America.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or ligand. Assembly can proceed by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a CAR LBD in complex with a co-regulator, optionally in further complex with a ligand. Manual model building using software such as QUANTATM or SYBYLTM typically follows.

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Useful programs to aid one of ordinary skill in the art in connecting the individual chemical entities or fragments include:

- 1. CAVEAT™ program (Bartlett *et al.*, 1989), which is available from the University of California, Berkeley, California, United States of America;
- 2. 3D Database systems, such as MACCS-3D™ system program, which is available from MDL Information Systems, San Leandro, California, United States of America. This area is reviewed in Martin, 1992; and
- 3. HOOK™ program (Eisen *et al.*, 1994), which is available from Accelrys Inc, San Diego, California, United States of America.

Instead of proceeding to build a NR LBD polypeptide ligand (in one embodiment a CAR LBD ligand) in a step-wise fashion one fragment or chemical entity at a time as described above, ligand compounds can be designed as a whole or *de novo* using the structural coordinates of a crystalline CAR LBD polypeptide of the present invention and either an empty binding site or optionally including some portion(s) of a known ligand(s). Applicable methods can employ the following software programs:

- LUDI™ program (Bohm, 1992), which is available from Accelrys Inc,
 San Diego, California, United States of America;
 - 2. LEGEND™ program (Nishibata & Itai, 1991); and
- 3. LEAPFROG™, which is available from Tripos Associates, St. Louis,
 30 Missouri, United States of America.

Other molecular modeling techniques can also be employed in accordance with this invention. See e.g., Cohen et al., 1990; Navia & Murcko,

-108-

1992; and U.S. Patent No. 6,008,033 to <u>Abdel-Meguid et al.</u>, all of which are incorporated herein by reference.

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Once a compound has been designed or selected by the above methods, the efficiency with which that compound can bind to a NR LBD can be tested and optimized by computational evaluation. By way of a particular example, a compound that has been designed or selected to function as a CAR LBD ligand can traverse a volume not overlapping that occupied by the binding site when it is bound to its native ligand. Additionally, an effective NR LBD ligand can demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient NR LBD ligands can be designed with a deformation energy of binding of in one embodiment not greater than about 10 kcal/mole, and in another embodiment not greater than 7 kcal/mole. It is possible for NR LBD ligands to interact with the polypeptide in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the thermodynamic average energy of the conformations observed when the ligand binds to the polypeptide.

A compound designed or selected as binding to a NR LBD polypeptide (preferably a CAR polypeptide, more preferably a CAR LBD polypeptide) can be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target polypeptide. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole, and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the ligand and the polypeptide when the ligand is bound to a NR LBD preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include:

1. GAUSSIAN 98[™], which is available from Gaussian, Inc., Pittsburgh, Pennsylvania, United States of America;

- 2. AMBER™ program, version 6.0, which is available from the University of California, San Francisco, California, United States of America;
- 3. QUANTA™ program, which is available from Accelrys Inc, San Diego, California, United States of America;
- 4. CHARMM® program, which is available from Accelrys Inc, San Diego, California, United States of America; and

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4. INSIGHT II® program, which is available from Accelrys Inc, San Diego, California, United States of America.

These programs can be implemented using a suitable computer system. Other hardware systems and software packages will be apparent to those skilled in the art after review of the disclosure of the present invention presented herein.

Once a NR LBD modulating compound has been optimally selected or designed, as described above, substitutions can then be made in some of its atoms or side groups in order to improve or modify its binding properties. In some cases, initial substitutions might be conservative, e.g., the replacement group will have approximately the same size, shape, hydrophobicity, and charge as the original group. In other cases, the replacement group will have different properties as desired to make specific interactions with the protein. Such substituted chemical compounds can then be analyzed for efficiency of fit to a NR LBD binding site using the same computer-based approaches described in detail above.

X.C. Sterically Similar Compounds

A further aspect of the present invention is that sterically similar compounds can be formulated to mimic the key portions of a CAR LBD structure. Such compounds are functional equivalents. The generation of a structural functional equivalent can be achieved by the techniques of modeling and chemical design known to those of skill in the art and described herein. Modeling and chemical design of CAR and CAR LBD structural equivalents can be based on the structure coordinates of a crystalline CAR

-110-

LBD polypeptide of the present invention. It will be understood that all such sterically similar constructs fall within the scope of the present invention.

XI. CAR Polypeptides

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The generation of mutant and chimeric CAR polypeptides is also an aspect of the present invention. A chimeric polypeptide can comprise a CAR LBD polypeptide or a portion of a CAR LBD, (e.g. a CAR LBD) which is fused to a candidate polypeptide or a suitable region of the candidate polypeptide. Throughout the present disclosure it is intended that the term "mutant" encompass not only mutants of a CAR LBD polypeptide but chimeric proteins generated using a CAR LBD as well. It is thus intended that the following discussion of mutant CAR LBDs apply mutatis mutandis to chimeric CAR and CAR LBD polypeptides and to structural equivalents thereof.

In accordance with the present invention, a mutation can be directed to a particular site or combination of sites of a wild-type CAR LBD. For example, an accessory binding site or the binding pocket can be chosen for mutagenesis. Similarly, a residue having a location on, at or near the surface of the polypeptide can be replaced, resulting in an altered surface charge of one or more charge units, as compared to the wild-type CAR and CAR LBD. Alternatively, an amino acid residue in a CAR or a CAR LBD can be chosen for replacement based on its hydrophilic or hydrophobic characteristics.

Such mutants can be characterized by any one of several different properties as compared with the wild-type CAR LBD. For example, such mutants can have an altered surface charge of one or more charge units, or can have an increase in overall stability. Other mutants can have altered ligand specificity in comparison with, or a higher specific activity than, a wild type CAR or CAR LBD.

CAR and CAR LBD mutants of the present invention can be generated in a number of ways. For example, the wild-type sequence of a CAR or a CAR LBD can be mutated at those sites identified using this invention as desirable for mutation by employing oligonucleotide-directed mutagenesis or other conventional methods. Alternatively, mutants of a CAR or a CAR LBD

-111-

can be generated by the site-specific replacement of a particular amino acid with an unnaturally occurring amino acid. In addition, CAR or CAR LBD mutants can be generated through replacement of an amino acid residue, for example, a particular cysteine or methionine residue, with selenocysteine or selenomethionine. This can be achieved by growing a host organism capable of expressing either the wild type or mutant polypeptide on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

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Mutations can be introduced into a DNA sequence coding for a CAR or a CAR LBD using synthetic oligonucleotides. These oligonucleotides contain nucleotide sequences flanking the desired mutation sites. Mutations can be generated in the full-length DNA sequence of a CAR or a CAR LBD or in any sequence coding for polypeptide fragments of a CAR or a CAR LBD.

According to the present invention, a mutated CAR or CAR LBD DNA sequence produced by the methods described above, or any alternative methods known in the art, can be expressed using an expression vector. An expression vector, as is well known to those of skill in the art, typically includes elements that permit autonomous replication in a host cell independent of the host genome, and one or more phenotypic markers for selection purposes. Either prior to or after insertion of the DNA sequences surrounding the desired CAR or CAR LBD mutant coding sequence, an expression vector includes control sequences encoding a promoter, operator, ribosome binding site, translation initiation signal, and, optionally, a repressor gene or various activator genes and a signal for termination. Where secretion of the produced mutant is desired, nucleotides encoding a "signal sequence" can be inserted prior to a CAR or a CAR LBD mutant coding sequence. For expression under the direction of the control sequences, a desired DNA sequence is operatively linked to the control sequences; that is, the sequence has an appropriate start signal in front of the DNA sequence encoding the CAR or CAR LBD mutant, and the correct reading frame to permit expression of that sequence under the control of the control sequences and production of the desired product encoded by that CAR or CAR LBD sequence.

-112-

Any of a wide variety of well-known available expression vectors can be used to express a mutated CAR or CAR LBD coding sequences of this invention. These include for example, vectors consisting of segments of chromosomal, non-chromosomal, and synthetic DNA sequences, such as known derivatives of SV40, known bacterial plasmids, e.g., plasmids from E. coli including colE1, pCR1, pBR322, pMB9 and their derivatives, wider host range plasmids, e.g., RP4, phage DNAs, e.g., derivatives of phage λ , e.g., NM 989, and other DNA phages, e.g., M13 and filamentous single stranded DNA phages, yeast plasmids and vectors derived from combinations of plasmids and phage DNAs, such as plasmids which have been modified to employ phage DNA or other expression control sequences. In one embodiment of the present invention, a vector amenable to expression in a pRSETA-based expression system is employed. The pRSETA expression system is available from Invitrogen, Inc., Carlsbad, California, United States of America.

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In addition, any of a wide variety of expression control sequences – *i.e.* sequences that control the expression of a DNA sequence when operatively linked to it – can be used in these vectors to express the mutated DNA sequences according to this invention. Such useful expression control sequences, include, but are not limited to the early and late promoters of SV40 for animal cells; the lac system, the trp system, the TAC or TRC system, the major operator and promoter regions of phage λ , and the control regions of fd coat protein for *E. coli*; the promoter for 3-phosphoglycerate kinase or other glycolytic enzymes, the promoters of acid phosphatase, (for example, Pho5), and the promoters of the yeast α -mating factors for yeast; as well as other sequences known to control the expression of genes of prokaryotic or eukaryotic cells or their viruses, and various combinations thereof.

A wide variety of hosts can be employed for producing mutated CAR and CAR LBD polypeptides according to this invention. These hosts include, for example, bacteria, such as *E. coli*, *Bacillus*, and *Streptomyces*; fungi, such

-113-

as yeasts; animal cells, such as CHO and COS-1 cells; plant cells; insect cells, such as Sf9 cells; and transgenic host cells.

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It should be understood that not all expression vectors and expression systems function in the same way to express mutated DNA sequences of this invention, and to produce modified CAR and CAR LBD polypeptides or CAR or CAR LBD mutants. Neither do all hosts function equally well with the same expression system. One of skill in the art can, however, make a selection among these vectors, expression control sequences and hosts without undue experimentation and without departing from the scope of this invention. For example, an important consideration in selecting a vector will be the ability of the vector to replicate in a given host. The copy number of the vector, the ability to control that copy number, and the expression of any other proteins encoded by the vector, such as antibiotic markers, should also be considered.

In selecting an expression control sequence, a variety of factors should also be considered. These include, for example, the relative strength of the system, its controllability and its compatibility with the DNA sequence encoding a modified CAR or CAR LBD polypeptide of this invention, with particular regard to the formation of potential secondary and tertiary structures.

Hosts should be selected by consideration of their compatibility with the chosen vector, the toxicity of a modified CAR or CAR LBD to them, their ability to express mature products, their ability to fold proteins correctly, their fermentation requirements, the ease of purification of a modified CAR or CAR LBD and safety. Within these parameters, one of skill in the art can select various vector/expression control system/host combinations that will produce useful amounts of a mutant CAR or CAR LBD. A mutant CAR or CAR LBD produced in these systems can be purified by a variety of conventional steps and strategies, including those used to purify the wild type CAR or CAR LBD.

Once a CAR LBD mutation(s) has been generated in the desired location, such as an active site or dimerization site, the mutants can be tested for any one of several properties of interest. For example, mutants can be screened for an altered charge at physiological pH. This is determined by

-114-

measuring the mutant CAR or CAR LBD isoelectric point (pl) and comparing the observed value with that of the wild-type parent. Isoelectric point can be measured by gel-electrophoresis according to the method of Wellner, 1971. A mutant CAR or CAR LBD polypeptide containing a replacement amino acid located at the surface of the enzyme, as provided by the structural information of this invention, can lead to an altered surface charge and an altered pl.

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XI.A. Generation of an Engineered CAR LBD or CAR LBD Mutant

In an embodiment of the present invention, a unique CAR or CAR LBD polypeptide is generated. Such a mutant can facilitate purification and the study of the ligand-binding abilities of a CAR polypeptide.

As used in the following discussion, the terms "engineered CAR", "engineered CAR LBD", "CAR mutant", and "CAR LBD mutant" refers to polypeptides having amino acid sequences which contain at least one mutation in the wild-type sequence. The terms also refer to CAR and CAR LBD polypeptides which are capable of exerting a biological effect in that they comprise all or a part of the amino acid sequence of an engineered CAR or CAR LBD polypeptide of the present invention, or cross-react with antibodies raised against an engineered CAR or CAR LBD polypeptide, or retain all or some or an enhanced degree of the biological activity of the engineered CAR or CAR LBD amino acid sequence or protein. Such biological activity can include the binding of small molecules in general, and the binding of Compound 1, in particular.

The terms "engineered CAR LBD" and "CAR LBD mutant" also includes analogs of an engineered CAR LBD or CAR LBD polypeptide. By "analog" is intended that a DNA or polypeptide sequence can contain alterations relative to the sequences disclosed herein, yet retain all or some or an enhanced degree of the biological activity of those sequences. Analogs can be derived from genomic nucleotide sequences or from other organisms, or can be created synthetically. Those of skill in the art will appreciate that other analogs, as yet undisclosed or undiscovered, can be used to design and/or construct CAR LBD or CAR LBD mutant analogs. There is no need for

-115-

a CAR LBD or CAR LBD mutant polypeptide to comprise all or substantially all of the amino acid sequence of SEQ ID NOs: 2 or 4. Shorter or longer sequences can be employed in the invention; shorter sequences are herein referred to as "segments". Thus, the terms "engineered CAR LBD" and "CAR LBD mutant" also includes fusion, chimeric or recombinant CAR LBD or CAR LBD mutant polypeptides and proteins comprising sequences of the present invention. Methods of preparing such proteins are disclosed herein above and are known in the art.

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XI.A.1. Sequences That Are Substantially Identical to a CAR or CAR LBD Mutant Sequence of the Present Invention

Nucleic acids that are substantially identical to a nucleic acid sequence of a CAR or CAR LBD mutant of the present invention, e.g. allelic variants, genetically altered versions of the gene, etc., bind to a CAR or CAR LBD mutant sequence under stringent hybridization conditions. By using probes, particularly labeled probes of DNA sequences, one can isolate homologous or related genes. The source of homologous genes can be any organism, including, but not limited to primates; rodents, such as rats and mice; canines; felines; bovines; equines; yeast; and nematodes.

Among mammalian species, e.g. human and mouse, homologs can have substantial sequence similarity, i.e. at least 75% sequence identity between nucleotide sequences. Sequence similarity is calculated based on a reference sequence, which can be a subset of a larger sequence, such as a conserved motif, coding region, flanking region, etc. In one embodiment, a reference sequence is at least about 18 nucleotides (nt) long, in another embodiment at least about 30 nt long, and can extend to the complete sequence that is being compared. Algorithms for sequence analysis are known in the art, such as BLAST, described in Altschul et al., 1990.

Percent identity or percent similarity of a DNA or peptide sequence can be determined, for example, by comparing sequence information using the GAP computer program, available from the University of Wisconsin Genetics Computer Group (now part of Accelrys Inc, San Diego, California, United

-116-

States of America). The GAP program utilizes the alignment method of Needleman et al., 1970, as revised by Smith et al., 1981. Briefly, the GAP program defines similarity as the number of aligned symbols (i.e., nucleotides or amino acids) that are similar, divided by the total number of symbols in the shorter of the two sequences. The preferred parameters for the GAP program are the default parameters, which do not impose a penalty for end gaps. See e.g., Schwartz et al., 1979; Gribskov et al., 1986.

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The term "similarity" is contrasted with the term "identity". Similarity is defined as above; "identity", however, refers to a nucleic acid or amino acid sequence having the same amino acid at the same relative position in a given family member of a gene family. Homology and similarity are generally viewed as broader terms than the term identity. Biochemically similar amino acids, for example leucine/isoleucine or glutamate/aspartate, can be present at the same position — these are not identical per se, but are biochemically "similar." As disclosed herein, these are referred to as conservative differences or conservative substitutions. This differs from a conservative mutation at the DNA level, which changes the nucleotide sequence without making a change in the encoded amino acid, e.g. TCC to TCA, both of which encode serine.

As used herein, DNA analog sequences are "substantially identical" to specific DNA sequences disclosed herein if: (a) the DNA analog sequence is derived from coding regions of the nucleic acid sequence shown in SEQ ID NOs: 1 or 3; or (b) the DNA analog sequence is capable of hybridization with DNA sequences of (a) under stringent conditions and which encode a biologically active CAR or CAR LBD gene product; or (c) the DNA sequences are degenerate as a result of alternative genetic code to the DNA analog sequences defined in (a) and/or (b). Substantially identical analog proteins and nucleic acids will have between about 70% and 80%, preferably between about 81% to about 90% or even more preferably between about 91% and 99% sequence identity with the corresponding sequence of the native protein or nucleic acid. Sequences having lesser degrees of identity but comparable biological activity are considered to be equivalents.

-117-

As used herein, "stringent conditions" refers to conditions of high stringency, for example 6X SSC, 0.2% polyvinylpyrrolidone, 0.2% Ficoll, 0.2% bovine serum albumin, 0.1% sodium dodecyl sulfate, 100 μg/ml salmon sperm DNA and 15% formamide at 68°C. For the purposes of specifying additional conditions of high stringency, preferred conditions comprise a salt concentration of about 200 mM and temperature of about 45°C. One example of stringent conditions is hybridization in 4X SSC, at 65°C, followed by a washing in 0.1X SSC at 65°C for one hour. Another exemplary stringent hybridization scheme uses 50% formamide, 4X SSC at 42°C.

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In contrast, nucleic acids having sequence similarity are detected by hybridization under lower stringency conditions. Thus, sequence identity can be determined by hybridization under lower stringency conditions, for example, at 50°C or higher and 0.1X SSC (9 mM NaCl/0.9 mM sodium citrate) and the sequences will remain bound when subjected to washing at 55°C in 1X SSC.

XI.A.2. Complementarity and Hybridization to an Engineered CAR or CAR LBD Mutant Sequence

As used herein, the term "functionally equivalent codon" is used to refer to codons that encode the same amino acid, such as the ACG and AGU codons for serine. CAR or CAR LBD-encoding nucleic acid sequences comprising SEQ ID NOs: 1 and 3, which have functionally equivalent codons are covered by the present invention. Thus, when referring to the sequence examples presented in SEQ ID NOs: 1 and 3, applicants contemplate substitution of functionally equivalent codons into the sequence example of SEQ ID NOs: 1 and 3. Thus, applicants are in possession of amino acid and nucleic acids sequences which include such substitutions but which are not set forth herein in their entirety for convenience.

It will also be understood by those of skill in the art that amino acid and nucleic acid sequences can include additional residues, such as additional N-or C-terminal amino acids or 5' or 3' nucleic acid sequences, and yet still be essentially as set forth in one of the sequences disclosed herein, so long as

-118-

the sequence retains biological protein activity where polypeptide expression is concerned. The addition of terminal sequences particularly applies to nucleic acid sequences which can, for example, include various non-coding sequences flanking either of the 5' or 3' portions of the coding region or can include various internal sequences, *i.e.*, introns, which are known to occur within genes.

XI.B. Biological Equivalents

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The present invention envisions and includes biological equivalents of CAR or CAR LBD mutant polypeptide of the present invention. The term "biological equivalent" refers to proteins having amino acid sequences which are substantially identical to the amino acid sequence of a CAR LBD mutant of the present invention and which are capable of exerting a biological effect in that they are capable of binding a small molecule, binding a co-regulator, homo- or heterodimerizing or cross-reacting with anti-CAR or CAR LBD mutant antibodies raised against a mutant CAR or CAR LBD polypeptide of the present invention.

For example, certain amino acids can be substituted for other amino acids in a protein structure without appreciable loss of interactive capacity with, for example, structures in the nucleus of a cell. Since it is the interactive capacity and nature of a protein that defines that protein's biological functional activity, certain amino acid sequence substitutions can be made in a protein sequence (or the nucleic acid sequence encoding it) to obtain a protein with the same, enhanced, or antagonistic properties. Such properties can be achieved by interaction with the normal targets of the protein, but this need not be the case, and the biological activity of the invention is not limited to a particular mechanism of action. It is thus in accordance with the present invention that various changes can be made in the amino acid sequence of a CAR or CAR LBD mutant polypeptide of the present invention or its underlying nucleic acid sequence without appreciable loss of biological utility or activity.

-119-

Biologically equivalent polypeptides, as used herein, are polypeptides in which certain, but not most or all, of the amino acids can be substituted. Thus, when referring to the sequence examples presented in SEQ ID NOs: 2 and 4, applicants envision substitution of codons that encode biologically equivalent amino acids, as described herein, into the sequence example of SEQ ID NOs: 2 and 4, respectively. Thus, applicants are in possession of amino acid and nucleic acids sequences which include such substitutions but which are not set forth herein in their entirety for convenience.

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Alternatively, functionally equivalent proteins or peptides can be created via the application of recombinant DNA technology, in which changes in the protein structure can be engineered, based on considerations of the properties of the amino acids being exchanged, e.g. substitution of Ile for Leu. Changes designed by man can be introduced through the application of site-directed mutagenesis techniques, e.g., to introduce improvements to the antigenicity of the protein or to test a CAR or CAR LBD mutant polypeptide of the present invention in order to modulate co-regulator-binding or other activity, at the molecular level.

Amino acid substitutions, such as those which might be employed in modifying a CAR or CAR LBD mutant polypeptide of the present invention are generally, but not necessarily, based on the relative similarity of the amino acid side-chain substituents, for example, their hydrophobicity, hydrophilicity, charge, size, and the like. An analysis of the size, shape and type of the amino acid side-chain substituents reveals that arginine, lysine and histidine are all positively charged residues; that alanine, glycine and serine are all of similar size; and that phenylalanine, tryptophan and tyrosine all have a generally similar shape. Therefore, based upon these considerations, arginine, lysine and histidine; alanine, glycine and serine; and phenylalanine, tryptophan and tyrosine; are defined herein as biologically functional equivalents. Those of skill in the art will appreciate other biologically functional equivalent changes. It is implicit in the above discussion, however, that one of skill in the art can appreciate that a radical, rather than a conservative substitution is warranted in a given situation. Non-conservative

-120-

substitutions in mutant CAR or CAR LBD polypeptides of the present invention are also an aspect of the present invention.

In making biologically functional equivalent amino acid substitutions, the hydropathic index of amino acids can be considered. Each amino acid has been assigned a hydropathic index on the basis of their hydrophobicity and charge characteristics, these are: isoleucine (+ 4.5); valine (+ 4.2); leucine (+ 3.8); phenylalanine (+ 2.8); cysteine (+ 2.5); methionine (+ 1.9); alanine (+ 1.8); glycine (-0.4); threonine (-0.7); serine (-0.8); tryptophan (-0.9); tyrosine (-1.3); proline (-1.6); histidine (-3.2); glutamate (-3.5); glutamine (-3.5); aspartate (-3.5); asparagine (-3.5); lysine (-3.9); and arginine (-4.5).

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The importance of the hydropathic amino acid index in conferring interactive biological function on a protein is generally understood in the art (Kyte & Doolittle, 1982, incorporated herein by reference). It is known that certain amino acids can be substituted for other amino acids having a similar hydropathic index or score and still retain a similar biological activity. In making changes based upon the hydropathic index, the substitution of amino acids whose hydropathic indices are within ±2 of the original value is preferred, those within ±1 of the original value are particularly preferred.

It is also understood in the art that the substitution of like amino acids can be made effectively on the basis of hydrophilicity. U.S. Patent No. 4,554,101, incorporated herein by reference, states that the greatest local average hydrophilicity of a protein, as governed by the hydrophilicity of its adjacent amino acids, correlates with its immunogenicity and antigenicity, *i.e.* with a biological property of the protein. It is understood that an amino acid can be substituted for another having a similar hydrophilicity value and still obtain a biologically equivalent protein.

As detailed in U.S. Patent No. 4,554,101 to <u>Hopp</u>, the following hydrophilicity values have been assigned to amino acid residues: arginine (+ 3.0); lysine (+ 3.0); aspartate (+ 3.0 ± 1); glutamate (+ 3.0 ± 1); serine (+ 0.3); asparagine (+ 0.2); glutamine (+ 0.2); glycine (0); threonine (-0.4); proline (- 0.5 ± 1); alanine (-0.5); histidine (-0.5); cysteine (-1.0); methionine (-1.3); valine

-121-

(-1.5); leucine (-1.8); isoleucine (-1.8); tyrosine (-2.3); phenylalanine (-2.5); tryptophan (-3.4).

In making changes based upon similar hydrophilicity values, the substitution of amino acids whose hydrophilicity values are within ± 2 of the original value is preferred, those that are within ± 1 of the original value are particularly preferred, and those within ± 0.5 of the original value are even more particularly preferred.

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While discussion has focused on functionally equivalent polypeptides arising from amino acid changes, it will be appreciated that these changes can be effected by alteration of the encoding DNA, taking into consideration also that the genetic code is degenerate and that two or more codons can code for the same amino acid.

Thus, it will also be understood that this invention is not limited to the particular amino acid and nucleic acid sequences of SEQ ID NOs: 1-4. Recombinant vectors and isolated DNA segments can therefore variously include a CAR or CAR LBD mutant polypeptide-encoding region itself, include coding regions bearing selected alterations or modifications in the basic coding region, or include larger polypeptides which nevertheless comprise a CAR or CAR LBD mutant polypeptide-encoding regions or can encode biologically functional equivalent proteins or polypeptides which have variant amino acid sequences. Biological activity of a CAR or CAR LBD mutant polypeptide can be determined, for example, by employing binding assays known to those of skill in the art.

The nucleic acid segments of the present invention, regardless of the length of the coding sequence itself, can be combined with other DNA sequences, such as promoters, enhancers, polyadenylation signals, additional restriction enzyme sites, multiple cloning sites, other coding segments, polyhistidine encoding segments and the like, such that their overall length can vary considerably. It is therefore contemplated that a nucleic acid fragment of almost any length can be employed, with the total length preferably being limited by the ease of preparation and use in the intended recombinant DNA protocol. For example, nucleic acid fragments can be

prepared which include a short stretch complementary to a nucleic acid sequence set forth in SEQ ID NOs: 1 and 3, such as about 10 nucleotides, and which are up to 10,000 or 5,000 base pairs in length. DNA segments with total lengths of about 4,000, 3,000, 2,000, 1,000, 500, 200, 100, and about 50 base pairs in length are also useful.

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The DNA segments of the present invention encompass biologically functional equivalents of CAR or CAR LBD mutant polypeptides. Such sequences can arise as a consequence of codon redundancy and functional equivalency that are known to occur naturally within nucleic acid sequences and the proteins thus encoded. Alternatively, functionally equivalent proteins or polypeptides can be created via the application of recombinant DNA technology, in which changes in the protein structure can be engineered, based on considerations of the properties of the amino acids being exchanged. Changes can be introduced through the application of site-directed mutagenesis techniques, e.g., to introduce improvements to the antigenicity of the protein or to test variants of a CAR or CAR LBD mutant of the present invention in order to examine the degree of lipid-binding activity, or other activity at the molecular level. Various site-directed mutagenesis techniques are known to those of skill in the art and can be employed in the present invention.

The invention further encompasses fusion proteins and peptides wherein a CAR or CAR LBD mutant coding region of the present invention is aligned within the same expression unit with other proteins or peptides having desired functions, such as for purification or immunodetection purposes.

Recombinant vectors form important further aspects of the present invention. Particularly useful vectors are those in which the coding portion of the DNA segment is positioned under the control of a promoter. The promoter can be that naturally associated with a CAR gene, as can be obtained by isolating the 5' non-coding sequences located upstream of the coding segment or exon, for example, using recombinant cloning and/or PCR technology and/or other methods known in the art, in conjunction with the compositions disclosed herein.

-123-

In other embodiments, certain advantages can be gained by positioning the coding DNA segment under the control of a recombinant, or heterologous, promoter. As used herein, a recombinant or heterologous promoter is a promoter that is not normally associated with a CAR gene in its natural environment. Such promoters can include promoters isolated from bacterial, viral, eukaryotic, or mammalian cells. Naturally, it will be important to employ a promoter that effectively directs the expression of the DNA segment in the cell type chosen for expression. The use of promoter and cell type combinations for protein expression is generally known to those of skill in the art of molecular biology (See e.g., Sambrook & Russell, 2001, specifically incorporated herein by reference). The promoters employed can be constitutive or inducible and can be used under the appropriate conditions to direct high level expression of the introduced DNA segment, such as is advantageous in the large-scale production of recombinant proteins or peptides. One exemplary promoter system contemplated for use in high-level expression is a T7 promoter-based system.

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XII. The Role of the Three-Dimensional Structure of the CAR LDB in Solving Additional CAR Crystals

Because polypeptides can crystallize in more than one crystal form, the structural coordinates of a CAR LBD, or portions thereof, in complex with a co-regulator as provided by the present invention, are particularly useful in solving the structure of other crystal forms of CAR and the crystalline forms of other NRs and CARs. The coordinates provided in the present invention can also be used to solve the structure of CAR or CAR LBD mutants (such as those above), CAR LDB co-complexes, or the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of CAR.

One method that can be employed for the purpose of solving additional CAR crystal structures is molecular replacement. See generally, Rossmann, 1972. In the molecular replacement method, an unknown crystal form, whether it is another crystal form of a CAR or a CAR LBD, (i.e. a CAR or a

CAR LBD mutant), a CAR or a CAR LBD polypeptide in complex with another compound (i.e. a "co-complex") or the crystal of some other protein with significant amino acid sequence homology to any functional region of the CAR LBD (e.g. another NR), can be determined using the CAR LBD structure coordinates provided in Tables 2-3. This method provides an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information ab initio.

In addition, in accordance with this invention, CAR or CAR LBD mutants can be crystallized in complex with known modulators, such as a coregulator. The crystal structures of a series of such complexes can then be solved by molecular replacement and compared with that of wild-type CAR or the wild-type CAR LBD. Potential sites for modification within the various binding sites of the enzyme can thus be conveniently identified. This information provides an additional tool for identifying efficient binding interactions, for example, increased hydrophobic interactions between the CAR LBD and a chemical entity or compound.

All of the complexes referred to in the present disclosure can be studied using X-ray diffraction techniques (See e.g., Blundell & Johnson, 1985) and can be refined using computer software, such as the X-PLORTM program (Brünger, 1992; X-PLOR is available from Accelrys Inc, San Diego, California, United States of America). This information can thus be used to optimize known classes of CAR and CAR LBD ligands, and more importantly, to design and synthesize novel classes of CAR and CAR LBD ligands, including co-regulators.

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Examples

The following Examples have been included to illustrate exemplary modes of the invention. Certain aspects of the following Examples are described in terms of techniques and procedures found or contemplated by the present inventors to work well in the practice of the invention. These Examples are exemplified through the use of standard laboratory practices of the inventors. In light of the present disclosure and the general level of skill in

-125-

the art, those of skill will appreciate that the following Examples are intended to be exemplary only and that numerous changes, modifications, and alterations can be employed without departing from the spirit and scope of the invention.

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Example 1

Protein Expression and Purification

A DNA fragment encoding residues 103 - 348 of a human CAR polypeptide (GenBank Accession No. Z30425) was amplified by the polymerase chain reaction (PCR) with a commercial kit (Stratagene, La Jolla, California, United States of America). The 5' PCR primer included an Nterminal poly-histidine tag sequence (MKKGHHHHHHG; SEQ ID NO: 5) along with an Ndel endonuclease restriction site (CATATG), and the 3' PCR primer contained a BamHI restriction site (GGATCC). The PCR primers used were 5'-CGGCGCCCATATGAAAAAGGTCATCATCATCATCATCATGGTCCT GTGAACTGAGTAAGGAGCAAG-3' (SEQ ID NO: 6) and 5'-CGGCGCGCGGATCCTTAGCTGCAGATCTCCTGGAGCAGCGG 3' (SEQ ID NO: 7). The amplified DNA fragment was inserted downstream of a T7 promoter from the pRSETA vector (Invitrogen Corp., Carlsbad, California, United States of America) at the Ndel-BamHl enzyme restriction sites. E. coli cells BL21(DE3) transformed with the above expression vector were grown on a carbenicillin antibiotic agar plate (50 mg/L carbenicillin). A starter culture of 80 ml LB media (10 g/L Bacto-Tryptone, 5 g/L yeast extract, 5 g/L NaCl, QC with distilled water) with carbenicillin antibiotic (50 mg/L carbenicillin) was grown from one colony at 37°C, 250 rpm for four hours. Twelve 2 L shaker flasks with 1L LB media and carbenicillin antibiotic (50 mg/L carbenicillin) were inoculated with 5 ml of the starter culture. Cells were grown at 23°C, 250 rpm for 16 hours to an OD₆₀₀ of 2.0, and harvested by centrifugation. The pellet was completely resuspended with 20 ml extract buffer (150 mM NaCl. 50 mM imidazole pH 7.5) per liter of cells. The cells were sonicated for 5 minutes using a Sonicator Ultrasonic Processor XL-2015 (Heat Systems, Inc., Farmingdale, New York, United States of America) at 0°C. The lysed cells

-126-

were centrifuged at 40,000g for 40 minutes and the supernatant was loaded on a 50 ml Ni-agarose column. The column was washed with 250 ml Buffer A (50 mM imidazole pH 7.5, 150 mM NaCl), 100 ml of Buffer B (200 mM imidazole pH 7.5, 150 mM NaCl), and the protein eluted with a 300 ml gradient to Buffer B (500 mM imidazole pH 7.5, 150 mM NaCl). The peak, which eluted at 45% Buffer B, contained 60 mg of His-tagged CAR LBD protein.

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This protein was diluted 5-fold in 10 mM Tris-Cl pH 8.0 to reduce the NaCl concentration before loading the entire sample on a 50 ml SP Sepharose FASTFLOWTM column (Pharmacia Biotech, now part of Amersham Biosciences Corp., Piscataway, New Jersey, United States of America). The column was washed with 200 ml Buffer S-A (10 mM Tris-Cl pH 8.0, 30 mM NaCl, 5 mM DTT, 1 mM EDTA pH 8.0) and the His-tagged CAR protein was eluted from the column by running a 300 ml increasing NaCl concentration gradient of Buffer S-B (10 mM Tris-Cl pH 8.0, 500 mM NaCl, 5 mM DTT, 1 mM EDTA pH 8.0). Peak fractions containing the CAR protein were pooled together, protein was concentrated to 1 mg/ml in CENTRIPREP™ 30 units (Millipore Corp., Bedford, Massachusetts, United States of America) concentrators. The protein yield was 4 mg/L cells grown. The protein was aliquoted into 10 mg aliquots at 1.0 mg/ml and stored on ice.

The purified CAR LBD protein (10 mg) was complexed with Compound 1 (10 mM in DMSO) in a 1:5 molar ratio and incubated on ice for 1 hour. The CAR LBD/Compound 1 protein complex was concentrated to 4 mg/ml in a CENTRIPREP™ 30 units and stored on ice until needed for crystallization efforts.

Example 2

Crystallization and Data Collection

CAR/Compound 1 crystals were grown at 4°C in hanging drops containing 1 μ l of the protein-ligand solutions disclosed in Example 1, and 1 μ l of well buffer (100 - 400 mM sodium potassium tartrate, pH 7.1 - 7.4). Crystals grew to a size of 100-200 μ m within several weeks. Before data

-127-

collection, crystals were transiently mixed with the well buffer that contains an additional 14% ethylene glycol, 7% glycerol, and then flash frozen in liquid nitrogen.

Orthorhombic CAR/ligand crystals formed in the $P2_12_12_1$ space group, with a=82.3 Å, b = 116.8 Å, c = 131.9 Å. Each asymmetric unit contained four CAR LBDs and four ligands. The crystals had a solvent content of 40%.

Crystals were screened with a Rigaku R-Axis IV detector (Rigaku International Corp., Tokyo, Japan), and data sets were collected with a MAR CCD detector at the IMCA 17ID beam line at Argonne National Labs (Argonne, Illinois, United States of America). The observed reflections were reduced, merged, and scaled with DENZOTM and SCALEPACKTM software in the HKL2000 package (Otwinowski, 1993).

Example 3

Structure Determination and Refinement

Structures were determined by molecular replacement methods with the CCP4 AMORETM program (Collaborative Computational Project, 1994; Navaza, 1994) using the poly-alanine model of the conserved region of VDR LBD. Coordinates for this model are presented in Table 3.

The best fitting solution generated with the AMORE[™] program gave a correlation coefficiency of 30% and an R-factor of 50%. The phases generated from molecular replacement were extensively refined and improved with solvent flattening, histogram matching, and NCS as implemented in CCP4DM and DMMULTI programs (Cowtan, 1994). Model building proceeded with QUANTA[™] (available from Accelrys Inc, San Diego, California, United States of America), and refinement progressed with CNX (Brünger *et al.*, 1998), and involved multiple cycles of manual rebuilding.

The structure of CAR in complex with the antagonist Compound 1 was determined. The statistics of the structure are summarized in Table 1.

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-128-

Example 4

Computational Analysis

Surface area was calculated with the Connolly MS program (Connolly, 1983) and the MVP program (Lambert, 1997). The binding pocket volumes were calculated with the program GRASP (Nicholls *et al.*, 1991), using the program MVP to close openings to solvent. The sequence alignments were generated with the MVP program.

Example 5

10 <u>Antagonist Assays</u>

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Screening of synthetic compound libraries with the purified CAR LBD protein by a Fluorescence Resonance Energy Transfer (FRET) Ligand Sensing Assay (Parks et al., 1999) was conducted to identify molecules that alter the basal interaction between a coactivator peptide and the CAR LBD protein. Briefly, the purified human CAR LBD protein was biotinylated and labeled with streptavidin-conjugated fluorophore allophycocyanin. The labeled CAR LBD protein was incubated with a test compound and with a peptide that included the second LXXLL binding motif of the nuclear coactivator SRC-1 (GenBank Accession No. U59302; amino acids 676-700) that was labeled with europium chelate. Data were collected with a WALLAC VICTORTM fluorescence reader (available from PerkinElmer Life Sciences Inc., Boston, Massachusetts, United States of America) in a time resolved mode and the fluorescence ratio calculated. Compound 1 was identified from the screen to be an inverse agonist molecule that reduces the basal fluorescent signal indicating that the CAR LBD/SRC-1 interaction was reduced below background levels. Standard dose response curves were conducted with the CAR LBD protein plus Compound 1 and the EC₅₀ was determined to be 15 nM.

-129-

Example 6

Synthesis of Compound 1

2-(benzhydrylamino) - 1 - (2-phenylethyl) - 1H - benzimidazole-6carboxamide (Compound 1) was synthesized as follows. A solution of 3fluoro-4-nitrobenzoic acid (1.28 g; 6.9 mmol) in 10 mL anhydrous N,N-5 dimethylformamide was treated with [O-(7-azabenzotriazol-1-yl)-1,1,3,3tetramethyluronium hexafluoro-phosphate] (2.6 g; 6.9 mmol) followed by N,N-diisopropylethylamine (3.6 ml, 20.7 mmol). After shaking for 5 min, the mixture was added to polystyrene Rink amide AM resin (1.0 g; 0.69 mmol/g; 0.69 mmol), and the reaction was rotated at 25°C for 18 h. The reaction 10 solution was drained, and the resin was washed sequentially with N,Ndimethylformamide (3X), dichloromethane (3X), methanol (2X), and dichloromethane (3X). The dried resin was treated with 15.2 ml of a 0.5 M phenethylamine in N-methylpyrrolidinone solution then rotated at 70°C for 15 15 The cooled reaction was drained, and the resin was washed hours. sequentially with N,N-dimethylformamide (3X), dichloromethane (3X), methanol (2X), and dichloromethane (3X). The resin was treated with 3.8 ml of 2.0 M SnCl₂•dihydrate in N-methylpyrrolidinone solution and rotated at 25 C for 24 hours. The reaction was drained and the resin washed sequentially 20 with 30% ethylenediamine (3X), *N,N*-dimethylformamide (3X),dichloromethane (3X), methanol (2X), and dichloromethane (3X). The dried diamine resin was treated with 7.6 ml of a 0.5 M benzyhydryl isothiocyanate in N-methylpyrrolidinone solution and 7.6 ml of a 1.0 M diisopropylcarbodiimide in N-methylpyrrolidinone solution. After rotating at 80°C for 24 h the reaction 25 was cooled to 25°C, drained, and the resin was washed sequentially with N,Ndimethylformamide (3X), dichloromethane (3X), methanol (2X), and dichloromethane (3X). The resin was treated with 30 ml 95% trifluoroacetic acid (TFA) in water and rotated at 25°C for 3 hours. The resin was drained and washed with dichloromethane. The filtrate was concentrated in vacuo to 30 give an oil. The oil was redissolved in dichloromethane and the solution was washed twice with saturated sodium bicarbonate (NaHCO₃). The organic layer was dried (Na₂SO₄), filtered, and concentrated in vacuo. The crude

-130-

product was triturated with Et₂O/hexanes, and the solid was collected by filtration to give 333 mg (98% yield) of the title compound as an off-white solid: 1 H NMR (DMSO-d6, 400 MHz) δ 7.68 (m, 2 H), 7.63 (d, 1 H, J = 8.4), 7.54 (dd, 1 H, J = 8.0, 1.2), 7.40-7.00 (m, 17 H), 6.36 (d, 1 H, J = 8), 4.42 (t, 2 H, J = 7.4), 2.97 (t, 2 H, J = 7.4); MS (ESP+) m/e 447 (MH⁺).

Table 2

Atomic Structure Coordinate Data Obtained From

X-ray Diffraction From the Ligand-binding Domain of CAR

In Complex With Compound 1

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	MOTA	1	N	LEU A	120	34.417	18.787	67.312	1.00 5		N
	ATOM	2	CA	LEU A		34.298	17.304	67.212	1.00 4		C
	ATOM	3	С	LEU A	120	33.672	16.891	65.886	1.00 4		C
15	MOTA	4	0	LEU A	120	32.815	17.592	65.344	1.00 4	19.49	0
	MOTA	5	CB	LEU A	120	33.447	16.756	68.363		50.64	C
	MOTA	6	CG	LEU A	120	34.003	16.880	69.783		51.38	C
	MOTA	7	CD1	LEU A	120	32.969	16.374	70.777		51.56	С
	MOTA	8	CD2	LEU A		35.297	16.085	69.906	1.00 5		C
20	ATOM	9	N	ARG A	121	34.106	15.745	65.375		48.14	N
	MOTA	10	CA	ARG A	121	33.599	15.221	64.117	1.00 4		С
	MOTA	11	C	ARG A	121	33.113	13.790	64.314	1.00 4		C
	ATOM	12	0	ARG A	121	33.775	12.836	63.905	1.00		0
	ATOM	13	CB	ARG A	121	34.700	15.264	63.052		48.45	C
25	ATOM	14	CG	ARG A		35.233	16.664	62.790	1.00		С
	ATOM	15	CD	ARG A		36.430	16.655	61.852	1.00		С
	ATOM	16	NE	ARG A		36.100	16.133	60.529	1.00		N
	MOTA	17	CZ	ARG A		36.947	16.112	59.504	1.00		С
	MOTA	18	NH1	_		38.178	16.586	59.648		54.50	N
30	MOTA	19	NH2			36.563	15.620	58.334		54.12	N
	ATOM	20	N	PRO A		31.946	13.622	64.955	1.00		N
	MOTA	21	CA	PRO A		31.403	12.282	65.187	1.00		C
	ATOM	22	С	PRO A		31.173	11.529	63.881	1.00		C
	ATOM	23	0	PRO A		30.823	12.125	62.862	1.00		0
35	MOTA	24	CB	PRO A		30.105	12.561	65.944		42.59	C
	ATOM	25	CG	PRO A		29.699	13.908	65.437		43.60	С
	MOTA	26	CD	PRO A		31.010	14.655	65.429	1.00		С
	MOTA	27	N	LYS A		31.379	10.218	63.920		41.53	N
40	MOTA	28	CA	LYS A		31.205	9.378	62.744		41.30	С
40	MOTA	29	С	LYS A		29.732	9.158	62.431		40.35	C
	MOTA	30	0	LYS A		28.877	9.250	63.313		39.21	0
	MOTA	31	CB	LYS A		31.885	8.024	62.965		42.56	C
	ATOM	32	CG	LYS A		33.371	8.127	63.279		45.26	С
45	ATOM	33	CD	LYS A		33.979	6.761	63.564		46.98	С
45	MOTA	34	CE	LYS A		35.463	6.876	63.882		47.93	С
	MOTA	35	NZ	LYS A		36.066	5.558	64.225		49.23	N
	MOTA	36	N		124	29.439	8.879	61.165		39.48	N
	MOTA	37	CA		A 124	28.071	8.622	60.744		38.64	C
	ATOM	38	С	LEU A	A 124	27.606	7.325	61.384	1.00	38.41	С

-131-

	MOTA	39	0	LEU A	124	28.293	6.308	61.304	1.00		0
	MOTA	40	CB	LEU A	124	27.996	8.491	59.220	1.00		C
	ATOM	41	CG	LEU A	124	28.162	9.776	58.406	1.00		С
	ATOM	42		LEU A		28.401	9.438	56.941	1.00		С
5	MOTA	43	CD2	LEU A	124	26.922	10.633	58.564	1.00		C
	ATOM	44	N	SER A	125	26.448	7.362	62.029	1.00		N
	MOTA	45	CA	SER A		25.905	6.168	62.661	1.00		C
	MOTA	46	С	SER A		25.496	5.197	61.561	1.00		С
	MOTA	47	0	SER A		25.386	5.581	60.395		39.53	0
10	MOTA	48	CB	SER A		24.679	6.523	63.495		39.88	C
	ATOM	49	OG	SER A		23.619	6.951	62.660		40.18	0
	MOTA	50	N	GLU A		25.271	3.940	61.923		41.33	N
	MOTA	51	CA	GLU A		24.865	2.956	60.930		42.41	С
	MOTA	52	С	GLU A		23.535	3.385	60.314		41.49	C
15	MOTA	53	0	GLU A		23.313	3.207	59.115		41.40	0
	ATOM	54	СВ	GLU A		24.727	1.573	61.573		45.02	С
	MOTA	55	CG	GLU A		24.325	0.463	60.605		48.95	C
	MOTA	56	CD	GLU A		25.202	0.414	59.361		51.93	С
	MOTA	57	OE1			24.878	1.105	58.366		53.34	0
20	MOTA	58	OE2	GLU A		26.222	-0.308	59.379		53.64	0
	MOTA	59	N		A 127	22.659	3.960	61.133		40.27	N
•	ATOM	60	CA		A 127	21.358	4.412	60.650		39.52	C
	ATOM	61	C		A 127	21.512	5.550	59.647		37.38	C
0E	MOTA	62	0		A 127	20.814	5.594	58.630		36.24	0
25	MOTA	63	CB		A 127	20.481	4.891	61.807		41.53	C
	ATOM	64	CG		A 127	19.091	5.320	61.363		45.78	C
	MOTA	65	CD		A 127	18.236	5.832	62.504	1.00	47.87	C
	ATOM	66	OE1		A 127	18.572	6.890	63.075		49.93	0
30	ATOM	67	OE2		A 127	17.227	5.173	62.832	1.00		0
30	MOTA	68	N		A 128	22.420	6.473	59.939	1.00	34.92	N
	ATOM	69	CA		A 128	22.654	7.603	59.052	1.00	33.94	C
	MOTA	70	C		A 128 A 128	23.239	7.134 7.671	57.721 56.665	1.00	34.19 32.45	C
	MOTA	71 72	O CB		A 128	22.905 23.573	8.622	59.735	1.00	33.20	C
35	ATOM ATOM	73	CG		A 128	22.861	9.410	60.835	1.00	32.00	C
J J		74	CD		A 128	23.785	10.317	61.629	1.00	32.20	c
	ATOM ATOM	75		GLN		23.765	11.326	62.192		33.66	0
	ATOM	76	NE2		A 128	25.061	9.960	61.691			N
	ATOM	77	NEZ		A 129	24.101	6.124	57.768	1.00	33.75	N
40	ATOM	78	CA		A 129	24.692	5.591	56.545	1.00		C
70	ATOM	79	C		A 129	23.588	4.965	55.702		34.31	c
	ATOM	80	Ö		A 129	23.562	5.111	54.479		33.78	ō
	MOTA	81	СВ		A 129	25.747	4.531	56.874		37.89	Č
	MOTA	82	CG		A 129	26.977	5.078	57.579		42.41	C
45	ATOM	83	CD		A 129	27.983	3.995	57.929		45.15	C
. •	ATOM	84	OE:		A 129	28.998	4.261	58.575		46.46	0
	ATOM	85			A 129		2.766	57.504		46.27	N
	ATOM	86	N		A 130		4.270	56.370		33.44	N
	ATOM	87			A 130		3.614	55.703		34.05	C
50	ATOM	88	С		A 130		4.638	55.018	1.00	32.98	С
	ATOM	89			A 130		4.436	53.881	1.00	31.44	0
	ATOM	90		ARG	A 130		2.794	56.723	1.00	37.04	С
	ATOM	91		ARG	A 130	19.497	2.141	56.184	1.00	41.36	C
	MOTA	92			A 130		1.108	57.171	1.00	45.69	C
55	ATOM	93	NE	ARG	A 130	17.642		56.790	1.00	49.25	N
	ATOM	94			A 130			56.938		51.46	С
	ATOM	95	NH	1 ARG	A 130			57.465		52.76	N
	ATOM	96	NH	2 ARG	A 130	15.357	0.757	56.556	1.00	52.73	N

-132-

	MOTA	97	N	ILE A	131	20.367	5.735	55.712	1.00 31.16	N
	ATOM	98	CA	ILE A	131	19.519	6.790	55.158	1.00 30.41	C
	MOTA	99	С	ILE A	131	20.120	7.343	53.865	1.00 29.21	C
_	MOTA	100	0	ILE A	131	19.414	7.528	52.872	1.00 27.86	0
5	MOTA	101	CB	ILE A		19.334	7.945	56.177	1.00 31.61	C
	MOTA	102	CG1	ILE A	131	18.513	7.448	57.372	1.00 32.47	С
	ATOM	103	CG2	ILE A	131	18.657	9.138	55.507	1.00 31.13	С
	MOTA	104	CD1	ILE A	131	18.287	8.496	58.457	1.00 33.63	C
	MOTA	105	N	ILE A	132	21.424	7.601	53.876	1.00 28.81	N
10	MOTA	106	CA	ILE A	132	22.094	8.124	52.691	1.00 29.13	C
	MOTA	107	С	ILE A	132	22.029	7.115	51.544	1.00 29.37	С
	ATOM	108	0	ILE A	132	21.786	7.486	50.394	1.00 28.72	0
	MOTA	109	CB	ILE A	A 132	23.570	8.468	52.994	1,00 29.90	
	MOTA	110	CG1	ILE A	A 132	23.628	9.625	53.995	1.00 30.31	C
15	ATOM	111	CG2	ILE A	A 132	24.306	8.838	51.708	1.00 30.32	C
	MOTA	112	CD1	ILE A	A 132	25.027	9.997	54.432	1.00 31.33	C
	ATOM	113	N	ALA A	A 133	22.239	5.841	51.862	1.00 28.31	N
	ATOM	114	CA	ALA Z	A 133	22.203	4.785	50.851	1.00 27.51	C
	MOTA	115	С	ALA A	A 133	20.820	4.680	50.213	1.00 26.94	С
20	ATOM	116	0	ALA A	A 133	20.694	4.542	48.993	1.00 26.91	0
	MOTA	117	CB	ALA 2	A 133	22.587	3.454	51.479	1.00 27.94	C
	MOTA	118	N	ILE :	A 134	19.786	4.739	51.044	1.00 26.00	N
	ATOM	119	CA	ILE :	A 134	18.413	4.659	50.564	1.00 25.19	C
	MOTA	120	C	ILE .	A 134	18.090	5.832	49.643	1.00 24.84	C
25	MOTA	121	0	ILE .	A 134	17.490	5.651	48.585	1.00 23.10	0
	MOTA	122	CB	ILE	A 134	17.416	4.660	51.742	1.00 26.47	C
	MOTA	123	CG1	ILE	A 134	17.511	3.331	52.493	1.00 27.92	C
	MOTA	124	CG2	ILE	A 134	15.997	4.901	51.239	1.00 26.56	C
	ATOM	125	CD1	ILE	A 134	16.714	3.297	53.778	1.00 29.71	. С
30	MOTA	126	N	LEU	A 135	18.494	7.030	50.047	1.00 23.54	N
	ATOM	127	CA	LEU	A 135	18.228	8.220	49.242	1.00 23.28	3 C
	MOTA	128	C	LEU	A 135	18.987	8.217	47.914	1.00 22.05	C
	MOTA	129	0	LEU	A 135	18.454	8.656	46.894	1.00 21.44	1 0
	ATOM	130	CB	LEU	A 135	18.559	9.480	50.045	1.00 23.23	L C
35	ATOM	131	CG	LEU	A 135	17.644	9.754	51.246	1.00 24.5	7 C
	MOTA	132	CD1	LEU	A 135	18.057	11.076	51.900	1.00 26.4	C
	MOTA	133	CD2	LEU	A 135	16.185	9.820	50.789	1.00 25.50	
	MOTA	134	N		A 136	20.223	7.725	47.913	1.00 22.40	
	MOTA	135	CA	LEU	A 136	20.991	7.675	46.669	1.00 23.29	9 C
40	ATOM	136	С	LEU	A 136	20.302	6.721	45.705	1.00 23.50) C
	MOTA	137	0		A 136	20.191	6.996	44.512	1.00 23.3	
	ATOM	138	CB	LEU	A 136	22.424	7.194	46.920	1.00 24.6	O C
	ATOM	139	CG	LEU	A 136	23.395	8.196	47.549	1.00 25.5	6 C
	MOTA	140	CD:	LEU	A 136	24.740	7.518	47.798	1.00 26.6	
45	MOTA	141	CD	LEU	A 136	23.555	9.398	46.628	1.00 26.0	
	ATOM	142	N	ASP	A 137	19.845	5.591	46.232	1.00 23.8	
	MOTA	143	CA	ASP	A 137	19.156	4.589	45.427	1.00 23.9	
	MOTA	144	С		A 137		5.152	44.870	1.00 23.6	
	MOTA	145	0	ASP	A 137		4.943	43.697	1.00 22.7	
50	MOTA	146	CB		A 137		3.348	46.282	1.00 26.9	
	MOTA	147			A 137		2.266	45.524	1.00 31.1	
	MOTA	148			A 137		1.947	45.900	1.00 34.7	
	ATOM	149			A 137		1.734	44.552	1.00 34.1	
	ATOM	150			A 138		5.867	45.714	1.00 22.3	
55	ATOM	151			A 138		6.472	45.312	1.00 22.3	
	MOTA	152			A 138		7.435	44.157		
	MOTA	153			A 138		7.445		1.00 20.8	
	ATOM	154	СВ	ALA	A 138	15.213	7.219	46.487	1.00 23.0	4 C

-133-

	MOTA	155	N I	HIS A	139	17.107	8.249	44.263	1.00 21.0	
	MOTA	156	CA I	HIS A	139	17.408	9.202	43.208	1.00 21.2	
	MOTA	157		HIS A		17.814	8.511	41.905	1.00 21.6	
_	MOTA	158	0 1	HIS P	139	17.385	8.913	40.824	1.00 21.1	
5	MOTA	159	CB 1	HIS P	139	18.528	10.152	43.631	1.00 21.2	
	MOTA	160			139	18.730	11.288	42.680	1.00 22.5	3 C
	ATOM	161			139	19.955	11.593	42.126	1.00 25.4	
	MOTA	162	CD2	HIS A	139	17.850	12.173	42.157	1.00 19.4	9 C
	MOTA	163	CE1	HIS A	139	19.820	12.615	41.300	1.00 20.8	2 C
10	MOTA	164	NE2	HIS A	139	18.552	12.986	41.301	1.00 23.9	9 N
	MOTA	165	N	HIS A	140	18.650	7.479	42.005	1.00 21.5	
	MOTA	166	CA	HIS A	140	19.099	6.760	40.819	1.00 22.2	0 C
	ATOM	167	С	HIS A	140	17.947	6.088	40.082	1.00 21.9	5 C
	ATOM	168	0	HIS A	A 140	17.997	5.911	38.861	1.00 21.8	7 0
15	MOTA	169	СВ	HIS A	A 140	20.153	5.710	41.193	1.00 23.7	6 C
	MOTA	170	CG	HIS A	A 140	21.398	6.291	41.787	1.00 25.8	0 C
	ATOM	171	ND1	HIS A	A 140	21.803	7.585	41.546	1.00 27.2	6 N
	MOTA	172			A 140	22.341	5.745	42.591	1.00 26.2	2 C
	ATOM	173			A 140	22.942	7.814	42.176	1.00 26.0	
20	ATOM	174			A 140	23.291	6.714	42.817	1.00 27.7	
	ATOM	175	N		A 141	16.908	5.719	40.821	1.00 20.4	
	ATOM	176	CA		A 141	15.745	5.071	40.225	1.00 21.8	
	ATOM	177	C		A 141	14.746	6.078	39.665	1.00 21.3	
	ATOM	178	ŏ		A 141	13.916	5.730	38.832	1.00 22.4	
25	ATOM	179	СВ		A 141	15.031	4.203	41.265	1.00 23.2	
	ATOM	180	CG		A 141	15.804	2.960	41.668	1.00 26.8	
	ATOM	181	CD		A 141	15.080	2.209	42.771	1.00 30.0	
	ATOM	182	CE		A 141	15.781	0.902	43.093	1.00 33.0	
	ATOM	183	NZ		A 141	15.122	0.206	44.231	1.00 36.	
30	ATOM	184	N		A 142	14.840	7.325	40.107	1.00 20.0	
	ATOM	185	CA		A 142	13.893	8.348	39.664	1.00 20.	
	ATOM	186	C		A 142	14.440	9.502	38.833	1.00 20.	
	ATOM	187	ō		A 142	13.682	10.375	38.420	1.00 20.	
	ATOM	188	СВ		A 142	13.142	8.935	40.865	1.00 20.	
35	ATOM	189	OG1		A 142	14.081	9.474	41.805	1.00 18.	
	ATOM	190	CG2		A 142	12.326	7.850	41.546	1.00 19.	
	ATOM	191	N		A 143	15.747	9.520	38.595	1.00 20.	
	ATOM	192	CA		A 143		10.566	37.768	1.00 20.	
	ATOM	193	C		A 143		9.895	36.706	1.00 20.	
40	ATOM	194	ŏ		A 143		9.323	37.013	1.00 21.	
	ATOM	195	СВ		A 143		11.529	38.610	1.00 20.	
	ATOM	196			A 143				1.00 20.	
	ATOM	197			A 143			36.915	1.00 21.	
	ATOM	198			A 143			37.994	1.00 21.	
45	ATOM	199			A 143			36.170	1.00 21.	
	ATOM	200			A 143			37.253	1.00 20.	
	ATOM	201	CZ		A 143			36.347	1.00 22.	
	ATOM	202	ОН		A 143			35.612	1.00 21.	
	MOTA	203	N		A 144			35.461	1.00 20.	
50	MOTA	204	CA		A 144			34.326	1.00 21.	
-	MOTA	205	C		A 144			33.751	1.00 22.	
	ATOM	205	0		A 144				1.00 21.	
	ATOM	207	СВ		A 144					
	ATOM	208	CG		A 144				1.00 22.	
55		208			A 144				1.00 22.	
JJ	MOTA				A 144					
	MOTA	210			A 144					
	MOTA	211			A 143					
	MOTA	212	CA	PRO	A 14:	20.119	11.034	33.403	1.00 23	

-134-

	ATOM	213	С	PRO A	145	20.968	11.106	31.968	1.00	22.50	C
	MOTA	214	0	PRO A	145	21.754	11.906	31.451	1.00	23.61	0
	MOTA	215	CB	PRO A	145	22.026	10.620	34.225	1.00	23.45	C
	ATOM	216	CG	PRO A	145	21.809	9.150	34.297	1.00	24.95	C
5	MOTA	217	CD	PRO A	145	20.347	9.052	34.700		23.26	C
	MOTA	218	N	THR A	146	20.265	10.224	31.256		22.03	N
	MOTA	219	CA	THR A	146	20.364	10.192	29.796	1.00	21.95	C
	MOTA	220	С	THR A	146	19.174	10.907	29.155		22.52	C
	MOTA	221		THR A			11.177	27.953		22.17	0
10	MOTA	222	CB	THR A	A 140		8.750	29.233		21.96	C
	MOTA	223		THR A			8.099	29.395		21.08	0
	MOTA	224	CG2	THR A			7.949	29.956		23.14	C
	MOTA	225	N	TYR A			11.210	29.963		22.04	N
	MOTA	226	CA	TYR A			11.912	29.489		22.53	C
15	MOTA	227	С	TYR A			11.191	28.309		23.10	C
	MOTA	228	0	TYR I			11.821	27.393		23.05	0
	MOTA	229	CB	TYR I			13.350	29.093		23.34	C
	MOTA	230	CG	TYR .			14.049	30.150		23.73	С
	MOTA	231	CD1	TYR .			14.274	29.968		25.15	C
20	MOTA	232	CD2	TYR .			14.398	31.372		23.61	,C
	MOTA	233	CE1	TYR .			14.818	30.989		25.82	,C
	MOTA	234	CE2	TYR .			14.941	32.396		26.56	С
	MOTA	235	CZ	TYR			15.142	32.199		26.11	C
05	MOTA	236	ОН	TYR			15.619	33.237		29.64	0
25	MOTA	237	N	SER			9.862	28.355		23.29	N
	MOTA	238	CA	SER			9.046	27.278		23.65	C
	MOTA	239	C	SER			9.078	27.073		24.65	C
	ATOM	240	0	SER			8.650	26.024		24.62	0
20	MOTA	241	CB	SER			7.593	27.450		26.66	C
30	ATOM	242	OG	SER			7.006	28.614		29.82	0
	ATOM	243	N	ASP			9.576	28.048		22.99	N
	ATOM	244	CA	ASP			9.632	27.905		23.85	C
	ATOM	245	C	ASP			10.925	27.272		24.00	C
35	MOTA	246	0	ASP			11.008	26.879		24.41	0
33	ATOM	247	CB	ASP	A 14		9.488 8.114	29.263 29.872		24.47 27.05	C
	ATOM	248	CG OD1					29.072		26.86	o
	MOTA	249 250	OD1					31.105		26.29	o
	MOTA MOTA	251	N	_	A 15			27.171		24.31	N
40	ATOM	252	CA		A 15			26.646		25.09	C
40	ATOM	253	C		A 15			25.252		25.91	C
	MOTA	254	0		A 15			24.949		25.61	Ö
	ATOM	255	СВ		A 15			26.715		24.68	č
	ATOM	256	CG		A 15			28.121		25.17	Č
45	ATOM	257		PHE				29.187		25.54	C
	ATOM	258		PHE				28.374		26.43	C
	ATOM	259		PHE				30.484		25.74	Ċ
	ATOM	260		PHE				29.667		25.55	C
	ATOM	261	CZ		A 1			30.721		24.63	С
50	ATOM	262	N		A 1			24.404		27.60	N
	MOTA	263	CA		A 1			23.063		28.74	С
	ATOM	264	C		A 1			23.094		28.90	C
	MOTA	265	Ō		A 1					28.40	
	ATOM	266			A 1			22.154		31.34	
55	ATOM	267	SG		A 1					37.88	
	ATOM	268	N		A 1				1.00	27.55	
	ATOM	269			A 1					27.93	
	ATOM	270			A 1					27.73	
			_		-						

-135-

	MOTA	271	0	GLN A 152	5.633	12.202	24.590	1.00 28.51	0
	MOTA	272	CB	GLN A 152	7.602	10.021	25.473	1.00 29.61	C
	MOTA	273	CG	GLN A 152	8.312	8.724	25.123	1.00 33.35	С
	MOTA	274	CD	GLN A 152	8.121	7.650	26.173	1.00 36.62	C
5	MOTA	275		GLN A 152	6.995	7.260	26.478	1.00 39.37	0
	MOTA	276		GLN A 152	9.225	7.162	26.732	1.00 38.35	N
	MOTA	277	N	PHE A 153	7.469	13.395	25.115	1.00 25.45	N
	MOTA	278	CA	PHE A 153	6.705	14.597	25.439	1.00 25.30	C
40	MOTA	279	C	PHE A 153	6.261	15.273	24.151	1.00 25.61	C
10	MOTA	280	0	PHE A 153	6.799	14.998	23.071	1.00 24.69	0
	MOTA	281	СВ	PHE A 153	7.564	15.608	26.215	1.00 23.94	C
	MOTA	282	CG	PHE A 153	8.187	15.060	27.469	1.00 23.45	C
	MOTA	283		PHE A 153	9.332	15.654	27.990	1.00 22.75	C
4 6	ATOM	284	CD2	PHE A 153	7.654	13.949	28.116	1.00 23.40	C
15	MOTA	285		PHE A 153	9.948	15.146	29.133	1.00 23.18	C
	ATOM	286	CE2	PHE A 153	8.261	13.434	29.263	1.00 22.50	C
	ATOM	287	CZ	PHE A 153	9.414	14.037	29.769	1.00 22.91	C
	MOTA	288	N	ARG A 154	5.276	16.158	24.260	1.00 25.51	N
20	MOTA	289	CA	ARG A 154	4.842	16.902	23.092	1.00 26.08	C
20	MOTA	290	C	ARG A 154	6.094	17.673	22.689	1.00 27.20 1.00 26.99	C O
	ATOM	291	0	ARG A 154	6.824	18.184 17.830	23.542 23.449	1.00 26.73	C
	ATOM	292 293	CB	ARG A 154 ARG A 154	3.681 2.351	17.030	23.449	1.00 20.73	C
	MOTA	294	CD	ARG A 154	1.232	17.067	24.066	1.00 27.71	C
25	MOTA MOTA	295	NE	ARG A 154	1.347	18.138	25.509	1.00 27.71	N
20	MOTA	296	CZ	ARG A 154	0.497	18.839	26.248	1.00 28.47	c
	ATOM	297	NH1		-0.538	19.444	25.677	1.00 29.16	N
	ATOM	298	NH2		0.673	18.919	27.560	1.00 27.66	N
	ATOM	299	N	PRO A 155	6.368	17.757	21.384	1.00 27.28	N
30	ATOM	300	CA	PRO A 155	7.554	18.454	20.892	1.00 28.12	C
	MOTA	301	C	PRO A 155	7.709	19.929	21.217	1.00 28.41	Č
	ATOM	302	0	PRO A 155	6.733	20.676	21.291	1.00 27.77	0
	ATOM	303	CB	PRO A 155	7.491	18.206	19.388	1.00 28.83	С
	MOTA	304	CG	PRO A 155	6.020	18.191	19.130	1.00 29.19	C
35	MOTA	305	CD	PRO A 155	5.508	17.335	20.262	1.00 28.61	C
	ATOM	306	N	PRO A 156	8.956	20.361	21.437	1.00 28.25	N
	ATOM	307	CA	PRO A 156	9.202	21.768	21.739	1.00 29.56	C
	MOTA	308	С	PRO A 156	9.054	22.532	20.425	1.00 30.08	С
	MOTA	309	0	PRO A 156	9.483	22.054	19.371	1.00 30.96	0
40	MOTA	310	CB	PRO A 156	10.640	21.763	22.250	1.00 29.92	С
	MOTA	311	CG	PRO A 156	11.262	20.646	21.476	1.00 30.45	С
	MOTA	312	CD	PRO A 156	10.198		21.538	1.00 29.15	C
	ATOM	313	N	VAL A 157	8.417	23.693	20.489	1.00 30.75	N
45	MOTA	314	CA	VAL A 157	8.220	24.538	19.319	1.00 31.52	C
45	ATOM	315	C	VAL A 157	8.764	25.907	19.692	1.00 32.33	C
	ATOM	316	0	VAL A 157	8.361	26.482	20.698	1.00 33.09	0
	ATOM	317	CB	VAL A 157	6.727	24.663	18.962	1.00 31.97	C
	ATOM	318		l VAL A 157	6.544		17.825	1.00 32.48 1.00 32.24	C
5 0	ATOM	319		2 VAL A 157	6.177		18.573	1.00 32.24	N
50	MOTA	320	N	ARG A 158	9.681		18.885	1.00 35.83	C
	ATOM	321	CA	ARG A 158	10.289			1.00 38.44	c
	ATOM	322	C	ARG A 158	10.020 10.763			1.00 38.44	0
	ATOM	323		ARG A 158 ARG A 158	11.794			1.00 35.86	C
55	MOTA MOTA	324 325		ARG A 158	12.131				
55	ATOM	325			13.606				
	ATOM	327			13.000				
	ATOM	328			14.006				
		220		C A 130	T=.000				_

-136-

	MOTA	329		ARG A		13.658	23.450	21.192	1.00 3		N
	MOTA	330		ARG A		14.370	23.926	23.319	1.00 2		N
	MOTA	331	N	VAL A		8.949	29.531	18.284	1.00 4		N
~	MOTA	332	CA	VAL A		8.568	30.574	17.338	1.00 4	-	C
5	MOTA	333	C	VAL A		9.511	31.767	17.432	1.00 4		C
	MOTA	334	0	VAL A		10.170	31.968	18.451	1.00 4		0
	MOTA	335	CB	VAL A		7.135	31.066	17.607	1.00 4		C
	ATOM	336		VAL A		6.147	29.937	17.367	1.00 4		С
4.0	MOTA	337		VAL A		7.027	31.577	19.040	1.00 4		C
10	MOTA	338	N	ASN A		9.576	32.557	16.365	1.00 4		N
	MOTA	339	CA	ASN A		10.440	33.730	16.357	1.00 4		C
	MOTA	340	C	ASN A		9.876	34.768	17.320	1.00 4		C
	MOTA	341	0	ASN A		8.728	35.198	17.185	1.00 4		0
	MOTA	342	CB	ASN A		10.530	34.326	14.949	1.00 4		C
15	MOTA	343	CG	ASN A		11.017	33.322	13.921	1.00 4		C
	MOTA	344		ASN A		12.030	32.649	14.124	1.00 4		0
	MOTA	345	ND2	ASN A	160	10.298	33.218	12.808	1.00 4		N
	MOTA	346	N	ASP A		10.688	35.156	18.298	1.00 4		N
	MOTA	347	CA	ASP A	161	10.282	36.142	19.289	1.00	14.79	С
20	MOTA	348	C	ASP A	161	11.515	36.834	19.862	1.00	14.74	C
	MOTA	349	0	ASP A	161	11.679	36.939	21.077	1.00	44.64	0
	MOTA	350	CB	ASP A	161	9.483	35.463	20.406	1.00	44.26	C
	MOTA	351	CG	ASP A	161	9.101	36.421	21.515	1.00	44.34	С
_	MOTA	352	OD1	ASP A	161	8.640	37.540	21.201	1.00	43.26	0
25	MOTA	353	OD2	ASP A	161	9.258	36.054	22.700	1.00		0
	MOTA	354	N	GLY A	162	12.383	37.304	18.972	1.00	44.73	N
	ATOM	355	CA	GLY A	162	13.592	37.977	19.409	1.00	44.74	С
	MOTA	356	C	GLY A	162	13.292	39.196	20.261	1.00	44.56	С
	MOTA	357	0	GLY A	162	14.135	39.638	21.042	1.00	45.10	0
30	ATOM	358	N	GLY A	A 163	12.086	39.736	20.116	1.00	44.30	N
	MOTA	359	CA	GLY A	A 163	11.706	40.911	20.879	1.00	43.74	C
	MOTA	360	С	GLY 2	A 163	11.206	40.618	22.282	1.00	43.23	C
	MOTA	361	0	GLY 2	A 163	11.066	41.533	23.096	1.00	43.53	0
	MOTA	362	N	GLY 2	A 164	10.946	39.346	22.572	1.00	42.43	N
35	MOTA	363	CA	GLY 2	A 164	10.450	38.980	23.889	1.00	40.70	C
	MOTA	364	C	GLY 2	A 164	9.094	39.616	24.130	1.00	39.47	C
	ATOM	365	0	GLY .	A 164	8.812	40.125	25.222	1.00	40.10	0
	ATOM	366	N	SER .	A 216	8.256	39.587	23.099	1.00	36.82	N
	MOTA	367	CA	SER .	A 216	6.918	40.165	23.162	1.00	35.37	C
40	MOTA	368	С		A 216	5.965	39.359	24.032	1.00	34.15	C
	MOTA	369	0		A 216	5.653	38.213	23.721		32.50	0
	MOTA	370	CB	SER	A 216	6.329	40.277			35.39	C
	MOTA	371	OG	SER	A 216	4.958	40.634	21.812		35.41	0
	MOTA	372	N	VAL	A 217	5.495		25.116		33.39	N
45	MOTA	373	CA		A 217	4.563	39.301	26.013		33.22	C
	ATOM	374	С		A 217	3.299		25.251		32.19	С
	MOTA	375	0	VAL	A 217	2.783		25.399		31.92	0
	ATOM	376	CB	VAL	A 217					33.21	C
	ATOM	377	CG:	l VAL	A 217					35.52	С
50	MOTA	378	CG	2 VAL	A 217					35.70	C
	MOTA	379			A 218					31.30	N
	ATOM	380	CA	THR	A 218					30.58	С
	ATOM	381	C		A 218					30.30	С
	ATOM	382			A 218					30.29	0
55	ATOM	383			A 218					30.65	
	MOTA	384		1 THR	A 218					30.30	
	MOTA	385	CG	2 THR	A 218					31.23	
	ATOM	386	N	LEU	A 219	2.849	38.325	22.018	1.00	29.44	N

-137-

	ATOM	387	CA	LEU A	219	3.095	37.206	21.117	1.00 2	29.87	С
	ATOM	388	С	LEU A	219	3.260	35.905	21.894	1.00 2	29.21	C
	ATOM	389	0	LEU A	219	2.710	34.869	21.516	1.00 2	29.73	0
	MOTA	390	CB	LEU A	219	4.355	37.462	20.286	1.00	31.48	C
5	ATOM	391	CG	LEU A	219	4.778	36.321	19.352	1.00	33.59	C
	ATOM	392	CD1	LEU A	219	3.700	36.083	18.301	1.00	34.93	C
	MOTA	393	CD2	LEU A	219	6.100	36.676	18.690	1.00	35.57	C
	ATOM	394	N	GLU A		4.018	35.963	22.982	1.00	28.82	N
	ATOM	395	CA	GLU A	220	4.258	34.781	23.801	1.00	29.09	C
10	ATOM	396	С	GLU A	220	2.958	34.194	24.342	1.00	29.07	C
	ATOM	397	0	GLU A		2.757	32.983	24.297	1.00	27.80	0
	ATOM	398	СВ	GLU A		5.213	35.131	24.946	1.00		C
	ATOM	399	CG	GLU A		6.620	35.466	24.456	1.00	32.76	C
	ATOM	400	CD	GLU A		7.434	36.277	25.450	1.00		C
15	ATOM	401		GLU A		8.574	36.657	25.104	1.00		0
	ATOM	402	OE2	GLU A		6.944	36.541	26.569	1.00		Ö
	ATOM	403	N	LEU A		2.073	35.052	24.841	1.00		N
	ATOM	404	CA	LEU A		0.799	34.592	25.383	1.00		C
	ATOM	405	C	LEU A		-0.143	34.089	24.293		29.77	Č
20	ATOM	406	ō	LEU A		-0.923	33.165	24.516		30.04	ō
	ATOM	407	СВ	LEU A		0.125	35.714	26.181		30.05	č
	ATOM	408	CG	LEU A		0.743	36.046	27.544		31.65	Ċ
	ATOM	409		LEU A		0.065	37.278	28.138		32.22	Č
	ATOM	410		LEU A		0.588	34.850	28.482		31.89	Č
25	ATOM	411	N	SER A		-0.066	34.687	23.108		31.28	N
20	MOTA	412	CA	SER A		-0.931	34.272	22.011		32.25	c
	MOTA	413	C	SER A		-0.536	32.905	21.460		32.84	č
	MOTA	414	ŏ	SER A		-1.380	32.170	20.947		33.76	ŏ
	MOTA	415	СВ	SER A		-0.895	35.304	20.877		34.81	c
30	MOTA	416	OG	SER A		0.367	35.315	20.230		39.03	ŏ
00	ATOM	417	N	GLN A		0.742	32.558	21.584		31.84	N
	ATOM	418	CA	GLN A		1.234	31.288	21.063		31.75	c
	ATOM	419	C	GLN A		1.596	30.215	22.089		30.53	Ċ
	ATOM	420	Ö	GLN A		1.306	29.039	21.869		30.69	Ö
35	ATOM	421	СВ	GLN A		2.434	31.550	20.151		34.71	C
00	ATOM	422	CG	GLN A		2.066	32.296	18.873		38.65	C
	ATOM	423	CD	GLN A		3.275	32.719	18.065		42.46	C
	MOTA	424	OE1			3.154	33.114	16.903		45.44	Ö
	ATOM	425	NE2			4.450	32.652	18.679		44.57	N
40	MOTA	426	NEZ	LEU A		2.226	30.610	23.195		28.64	N
70	MOTA	427	CA	LEU A		2.632	29.654	24.232		27.07	C
						3.209		23.569		26.40	C
	ATOM	428	C	LEU A		2.898	27.274			25.81	
	MOTA	429	O CB	LEU A		1.424	29.276	23.962 25.102		27.70	O C
45	MOTA	430		LEU A			30.424	25.102			
45	ATOM	431	CG			0.785	29.931	26.615		27.88 29.53	C
	MOTA	432		L LEU A		-0.463		26.884		27.54	
	ATOM	433		LEU A		1.789	30.981			25.74	C
	ATOM	434	N	SER A		4.071	28.614 27.531	22.577 21.798		25.83	N N
EΩ	ATOM	435	CA	SER A		4.667					
50	ATOM	436	C	SER A		5.454	26.473	22.563		25.18	C
	MOTA	437		SER A		5.446	25.302	22.182		25.89	0
	ATOM	438	CB	SER A		5.557	28.110	20.696		26.31	C
	ATOM	439		SER A		6.710	28.731	21.233		29.36	0
E =	ATOM	440		MET A		6.132	26.880			24.58	
55	ATOM	441		MET A		6.931				24.51	
	MOTA	442		MET A		6.193				24.00	
	ATOM	443		MET A		6.725				24.19	
	MOTA	444	СВ	MET A	226	8.219	26.629	24.905	1.00	24.70	С

-138-

	MOTA	445	CG	MET A		9.329	26.715	23.870	1.00		С
	ATOM	446	SD	MET A		9.960	25.094	23.351	1.00		S
	ATOM	447	CE	MET A		10.773	24.531	24.858	1.00		С
_	ATOM	448	N	LEU A		4.969	25.850	25.872	1.00		N
5	ATOM	449	CA	LEŲ A		4.225	25.377	27.030	1.00		C
	MOTA	450	С	LEU A		3.882	23.887	27.032	1.00		C
	ATOM	451	0	LEU A		4.062	23.218	28.052	1.00		0
	ATOM	452	CB	LEU A		2.949	26.212	27.237	1.00		С
40	ATOM	453	CG	LEU A		2.139	25.868	28.494	1.00		C
10	ATOM	454		LEU A		3.019	25.994	29.730		25.75	C
	MOTA	455		LEU A		0.936	26.798	28.612		25.81	C
	MOTA	456	N	PRO A		3.395	23.336	25.901		24.00	N
	ATOM	457	CA	PRO A		3.073	21.904	25.931		23.78	C
4-	MOTA	458	С	PRO A		4.261	21.024	26.330		23.69	C
15	MOTA	459	0	PRO A		4.123	20.109	27.155		23.20	0
	ATOM	460	CB	PRO A		2.602	21.626	24.504		24.23	C
	ATOM	461	CG	PRO A		1.957	22.939	24.110		24.58	C
	MOTA	462	CD	PRO A		2.962	23.948	24.629		23.63	C
	MOTA	463	N	HIS A		5.421	21.305	25.747		22.38	N
20	MOTA	464	CA	HIS A		6.626	20.532	26.037		22.16	C
	MOTA	465	С	HIS A		7.089	20.679	27.490		21.32	C
	ATOM	466	0	HIS A		7.409	19.687	28.151		20.38	0
	MOTA	467	CB	HIS A		7.765	20.951	25.103		22.65	C
05	MOTA	468	CG	HIS A		9.037	20.196	25.337		23.54	C
25	MOTA	469		HIS A		9.235	18.910	24.883		24.88	N
	MOTA	470		HIS A		10.160	20.535	26.012		23.99	C
	ATOM	471		HIS A		10.427	18.488	25.270		25.42	C
	MOTA	472		HIS A		11.009	19.455	25.957		23.32	N
20	ATOM	473	N	LEU A		7.139	21.913	27.985		20.90	N
30	ATOM	474	CA	LEU A		7.578	22.139	29.355		21.22	C
	MOTA	475	C	LEU A		6.563	21.623	30.361		21.08	C
	MOTA	476	0	LEU A		6.938	21.164	31.435		19.50	0
	MOTA	477	CB	LEU A		7.858	23.625	29.602		21.98	С
25	MOTA	478	CG	LEU A		9.051	24.211	28.839		23.32	С
35	ATOM	479	CD1			9.285	25.637	29.322		25.98	C
	ATOM	480		LEU A		10.311	23.371	29.073		24.89	С
	ATOM	481	N	ALA A		5.279	21.703	30.022	1.00		N
	MOTA	482	CA	ALA A		4.243	21.197	30.917		21.50	C
40	ATOM	483	C	ALA A		4.421	19.685	31.040		21.12	C
40	MOTA	484	0_	ALA A		4.303	19.124	32.129		21.78	0
	MOTA	485	СВ	ALA A		2.859	21.522	30.361		22.95	С
	MOTA	486	N	ASP A		4.707				20.87	
	ATOM	487	CA	ASP A		4.910	17.582	29.916		21.48	C
45	ATOM	488	C	ASP A		6.168	17.228	30.711		20.43	C
45	ATOM	489	0	ASP A		6.167	16.259	31.463		21.59	0
	ATOM	490	CB	ASP A		5.022	17.056	28.482		21.87	C
	MOTA	491	CG	ASP A		3.664	16.893	27.807		25.14	C
	MOTA	492		ASP A		3.639	16.665	26.582		26.65	0
50	ATOM	493		ASP A		2.623	16.982	28.497		25.49	0
30	ATOM	494	N	LEU A		7.228	18.018	30.549		21.20	N
	ATOM	495	CA	LEU A		8.483	17.785	31.278		20.50	C
	ATOM	496	C	LEU A		8.267	17.940	32.785		20.58	C
	MOTA	497	0	LEU A		8.755	17.139	33.587		18.39	0
55	MOTA	498	CB	LEU A		9.565	18.770	30.811		20.92	С
33	MOTA	499	CG	LEU A						20.96	
	MOTA	500		LEU A						22.15	
	MOTA	501		LEU A			19.969			22.47	
	ATOM	502	N	VAL A	A 234	7.539	18.981	33.172	1.00	20.09	N

-139-

	ATOM	503	CA	VAL A 234	7.263	19.217	34.583	1.00 20.15	
	ATOM	504		VAL A 234	6.320	18.152	35.146	1.00 19.97	
	ATOM	505		VAL A 234	6.500	17.691	36.268		5
	ATOM	506	•	VAL A 234	6.665	20.630	34.796	1.00 21.02	
5	ATOM	507		VAL A 234	6.104	20.778	36.209		3
9	ATOM	508		VAL A 234	7.754	21.679	34.566		Š
	ATOM	509	N	SER A 235	5.324	17.749	34.362		N
	ATOM	510	CA	SER A 235	4.378	16.732	34.821		C
	MOTA	511	C	SER A 235	5.117	15.413	35.079		C
10	ATOM	512	0	SER A 235	4.906	14.743	36.095		Ö
10	MOTA	513	СВ	SER A 235	3.284	16.537	33.767		C
	ATOM	514	OG	SER A 235	2.229	15.734	34.274		0
	ATOM	515	N	TYR A 236	5.983	15.057	34.140		N
	ATOM	516	CA	TYR A 236	6.796	13.849	34.222		c
15	MOTA	517	C	TYR A 236	7.660	13.930	35.479		C
13	ATOM	518	0	TYR A 236	7.792	12.958	36.223		Õ
	ATOM	519	СВ	TYR A 236	7.675	13.781	32.976		Č
	ATOM	520	CG	TYR A 236	8.800	12.764	32.990		c
	MOTA	521	CD1		8.601	11.466	32.527		C
20	ATOM	522	CD2	TYR A 236	10.084	13.131	33.391		Č
20	ATOM	523		TYR A 236	9.665	10.557	32.448		c
	ATOM	524	CE2		11.149	12.233	33.321		č
	ATOM	525	CZ	TYR A 236	10.934	10.954	32.846		č
	ATOM	526	OH	TYR A 236	11.996	10.079	32.749		ŏ
25	ATOM	527	N	SER A 237	8.241	15.105	35.711		N
	ATOM	528	CA	SER A 237	9.106	15.312	36.868	1.00 18.19	c
	MOTA	529	C	SER A 237	8.373	15.218	38.199	1.00 18.73	Č
	ATOM	530	Ö	SER A 237	8.929	14.737	39.184	1.00 19.34	ō
	MOTA	531	СВ	SER A 237	9.830	16.654	36.730	1.00 18.72	Č
30	ATOM	532	OG	SER A 237	10.648	16.628	35.573	1.00 19.76	ō
•	ATOM	533	N	ILE A 238	7.128	15.680	38.237	1.00 18.89	N
	ATOM	534	CA	ILE A 238	6.343	15.597	39.460	1.00 20.25	C
	ATOM	535	C	ILE A 238	6.101	14.119	39.759	1.00 20.17	Ċ
	ATOM	536	ō	ILE A 238	6.129	13.705	40.914	1.00 20.62	Ō
35	ATOM	537	СВ	ILE A 238	4.984	16.337	39.317	1.00 21.21	C
	ATOM	538	CG1		5.226	17.847	39.236	1.00 23.61	C
	ATOM	539	CG2		4.068	16.001	40.502	1.00 23.76	С
	ATOM	540	CD1		3.972	18.668	38.937	1.00 24.70	C
	MOTA	541	N	GLN A 239	5.868	13.315	38.719	1.00 20.04	N
40	ATOM	542	CA	GLN A 239	5.657	11.890	38.936	1.00 19.72	С
	ATOM	543	С	GLN A 239	6.911	11.261	39.531	1.00 20.24	С
	ATOM	544	O	GLN A 239	6.823	10.433		1.00 19.92	0
	ATOM	545	СВ	GLN A 239	5.288	11.178	37.628	1.00 21.35	С
	ATOM	546	CG	GLN A 239	3.920	11.576		1.00 21.87	С
45	ATOM	547	CD	GLN A 239	3.487	10.707	35.922	1.00 23.58	С
	ATOM	548	OE1	L GLN A 239	3.092	9.556	36.105	1.00 26.39	0
	ATOM	549		2 GLN A 239	3.568	11.249	34.720	1.00 22.31	N
	ATOM	550	N	LYS A 240	8.080	11.661	39.037	1.00 19.37	N
	ATOM	551	CA	LYS A 240	9.336	11.116	39.557	1.00 19.49	С
50	ATOM	552	С	LYS A 240	9.575	11.583	40.994	1.00 20.03	C
	ATOM	553	0	LYS A 240					0
	ATOM	554	СВ	LYS A 240					С
	ATOM	555		LYS A 240					С
	ATOM	556		LYS A 240	10.174	9.491	37.165	1.00 20.85	С
55	ATOM	557		LYS A 240	10.201			1.00 20.78	С
	ATOM	558		LYS A 240	9.919				N
	MOTA	559	N	VAL A 241	9.203	12.827			N
	MOTA	560	CA	VAL A 241	9.355	13.380	42.630	1.00 21.18	С

-140-

	MOTA	561	C	VAL A 241	8.466	12.633	43.621	1.00 22.58	C
	MOTA	562	0	VAL A 241	8.845	12.418	44.769	1.00 22.01	0
	MOTA	563	CB	VAL A 241	9.006	14.890	42.658	1.00 22.53	C
	MOTA	564		VAL A 241	8.893	15.392	44.104	1.00 23.49	C
5	MOTA	565	CG2	VAL A 241	10.092	15.671	41.929	1.00 22.43	C
	MOTA	566	N	ILE A 242	7.277	12.237	43.178	1.00 22.44	N
	ATOM	567	CA	ILE A 242	6.375	11.492	44.052	1.00 23.64	C
	ATOM	568	C	ILE A 242	7.027	10.157	44.416	1.00 23.45	C
	MOTA	569	0	ILE A 242	6.987	9.726	45.573	1.00 25.50	0
10	ATOM	570	СВ	ILE A 242	5.012	11.255	43.360	1.00 24.32	C
	ATOM	571	CG1	ILE A 242	4.235	12.575	43.303	1.00 25.64	C
	MOTA	572	CG2	ILE A 242	4.214	10.186	44.104	1.00 24.95	C
	MOTA	573	CD1	ILE A 242	3.012	12.540	42.401	1.00 25.41	C
	ATOM	574	N	GLY A 243	7.652	9.521	43.431	1.00 22.76	N
15	ATOM	575	CA	GLY A 243	8.310	8.246	43.665	1.00 23.14	C
	MOTA	576	С	GLY A 243	9.491	8.385	44.604	1.00 23.29	C
	ATOM	577	0	GLY A 243	9.719	7.525	45.454	1.00 24.26	0
	ATOM	578	N	PHE A 244	10.244	9.471	44.443	1.00 22.21	N
	ATOM	579	CA	PHE A 244	11.406	9.754	45.287	1.00 23.08	C
20	ATOM	580	C	PHE A 244	10.962	9.960	46.734	1.00 23.33	C
	ATOM	581	0	PHE A 244	11.509	9.359	47.665	1.00 22.96	0
	ATOM	582	CB	PHE A 244	12.110	11.023	44.799	1.00 21.55	C
	ATOM	583	CG	PHE A 244	13.264	11.454	45.663	1.00 23.20	C
	ATOM	584	CD1	PHE A 244	14.474	10.764	45.632	1.00 25.04	C
25	MOTA	585	CD2	PHE A 244	13.140	12.548	46.516	1.00 24.78	C
	ATOM	586	CE1		15.542	11.157	46.437	1.00 25.46	C
	ATOM	587	CE2		14.205	12.950	47.327	1.00 24.71	C
	ATOM	588	CZ	PHE A 244	15.407	12.254	47.286	1.00 24.22	C
	ATOM	589	N	ALA A 245	9.963	10.819	46.912	1.00 23.25	N
30	ATOM	590	CA	ALA A 245	9.441	11.134	48.233	1.00 23.37	C
	ATOM	591	C	ALA A 245	8.960	9.906	49.006	1.00 25.09	C
	ATOM	592	Ō	ALA A 245	9.182	9.805	50.212	1.00 24.87	0
	ATOM	593	СВ	ALA A 245	8.310	12.156	48.113	1.00 22.36	С
	ATOM	594	N	LYS A 246	8.309	8.975	48.314	1.00 26.15	N
35	MOTA	595	CA	LYS A 246	7.800	7.768	48.959	1.00 28.66	C
	ATOM	596	C	LYS A 246	8.914	6.918	49.562	1.00 29.21	C
	ATOM	597	0	LYS A 246	8.668	6.117	50.466	1.00 29.75	0
	MOTA	598	СВ	LYS A 246	6.997	6.931	47.957	1.00 30.93	C
	ATOM	599	CG	LYS A 246	5.702	7.593	47.501	1.00 34.75	
40	MOTA	600	CD	LYS A 246	5.017	6.811	46.383	1.00 37.28	
	MOTA	601	CE	LYS A 246	4.410	5.501	46.873	1.00 40.02	С
	ATOM	602	NZ	LYS A 246	3.230	5.724		1.00 42.15	N
	MOTA	603	N	MET A 247	10.138	7.104	49.074	1.00 28.68	N
	MOTA	604	CA	MET A 247	11.282	6.339	49.562	1.00 29.45	C
45	MOTA	605	С	MET A 247	12.076	7.021	50.681	1.00 28.75	
	ATOM	606	0	MET A 247	13.012	6.431	51.230	1.00 28.61	0
	ATOM	607	CB	MET A 247	12.219	5.990	48.396	1.00 30.97	
	MOTA	608	CG	MET A 247	11.614	5.007	47.393	1.00 34.76	
	ATOM	609	SD	MET A 247	12.766	4.475	46.096	1.00 39.72	
50	ATOM	610	CE	MET A 247	12.303	5.554	44.763	1.00 39.07	
	ATOM	611	N	ILE A 248	11.709	8.253	51.023	1.00 27.31	
	ATOM	612	CA	ILE A 248	12.391	8.973	52.100	1.00 28.07	
	ATOM	613	C	ILE A 248	12.033	8.295	53.420		
	ATOM	614		ILE A 248	10.859	8.179	53.763	1.00 28.97	
55	ATOM	615	СВ	ILE A 248	11.934		52.195		
	ATOM	616			12.299		50.916		
	MOTA	617		2 ILE A 248					
	MOTA	618		1 ILE A 248					
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-141-

	ATOM	619		PRO A		13.041	7.844	54.181	1.00		N
	MOTA	620		PRO A		12.764	7.182	55.460	1.00		C
	ATOM	621	С	PRO A		11.818	7.992	56.348	1.00		С
_	MOTA	622	0	PRO A		12.107	9.138	56.688	1.00		0
5	MOTA	623	CB	PRO A		14.153	7.035	56.075	1.00		C
	MOTA	624	CG	PRO A		15.021	6.835	54.871	1.00		C
	MOTA	625	CD	PRO A		14.490	7.890	53.917	1.00		C
	MOTA	626	N	GLY A		10.686	7.392	56.706	1.00		N
	MOTA	627	CA	GLY A		9.725	8.064	57.565	1.00		С
10	ATOM	628	С	GLY A		8.542	8.700	56.858	1.00		C
	ATOM	629	0	GLY A		7.484	8.888	57.459	1.00		0
	MOTA	630	N	PHE A		8.709	9.023	55.579	1.00		N
	MOTA	631	CA	PHE A		7.643	9.658	54.809	1.00		С
	MOTA	632	С	PHE A		6.335	8.871	54.833		34.57	C
15	MOTA	633	0	PHE A		5.259	9.455	54.964		35.10	0
	MOTA	634	CB	PHE A		8.082	9.850	53.356		31.35	C
	MOTA	635	CG	PHE A		7.180	10.754	52.564		29.89	C
	ATOM	636		PHE A		7.234	12.134	52.735			C
	ATOM	637	CD2	PHE A		6.276	10.227	51.643		30.05	C
20	ATOM	638		PHE A		6.400	12.979	51.999			C
	ATOM	639	CE2	PHE A		5.441	11.063	50.906		28.78	С
	ATOM	640	CZ		A 251	5.505	12.440	51.085		28.48	С
	MOTA	641	N		A 252	6.431	7.551	54.703		36.83	N
	MOTA	642	CA		A 252	5.250	6.691	54.698		39.19	C
25	MOTA	643	C		A 252	4.535	6.647	56.045		39.61	C
	MOTA	644	0		A 252	3.391	6.200	56.127		40.31	0
	MOTA	645	CB		A 252	5.625	5.262	54.292		41.06	C
	MOTA	646	CG		A 252	6.138	5.101	52.867		44.96	C
	MOTA	647	CD		A 252	6.260	3.620	52.516		47.63	С
30	MOTA	648	NE		A 252	6.777	3.393	51.169		50.79	N
	ATOM	649	CZ		A 252	8.062	3.459	50.831		51.79	C
	ATOM	650	NH1		A 252	8.982	3.745	51.745		52.82	N
	MOTA	651		ARG		8.427	3.235	49.576		52.64	N
0.5	MOTA	652	N		A 253	5.205	7.102	57.098	1.00		N
35	MOTA	653	CA		A 253	4.610	7.097	58.430		40.45	C
	ATOM	654	C		A 253	3.648	8.255	58.635		39.90	C
	MOTA	655	0		A 253	2.902	8.284	59.612			0
	MOTA	656	CB		A 253	5.698	7.127	59.506			C
40	ATOM	657	CG		A 253	6.524	5.856	59.531		44.84	C
40	MOTA	658			A 253	5.938	4.767	59.345		47.60	0
	ATOM	659			A 253	7.752	5.942	59.743		45.66	0
	MOTA		N		A 254	3.669				38.00	
	MOTA	661	CA		A 254	2.782	10.361	57.780		37.81	C
AE	ATOM	662	C		A 254	1.417	9.978	57.218		37.76	C
45	MOTA	663	0		A 254	1.293	9.000	56.476		37.49	0
	MOTA	664	CB		A 254	3.348	11.521	56.955		36.51	C
	MOTA	665	CG		A 254		12.101	57.346		36.86	C
	ATOM	666			A 254		13.113	56.297		35.66	C
EΛ	ATOM	667			A 254		12.751	58.719		36.85	C
50	MOTA	668	N		A 255		10.745	57.579		38.14	N
	ATOM	669	CA		A 255		10.496			39.08	C
	MOTA	670	С		A 255		10.828			39.76	C
	ATOM	671	0		A 255		11.593			39.15	
E.E.	ATOM	672	CB		A 255		11.397			39.68	
55	ATOM	673			A 255		12.767			39.47	
	ATOM	674			A 255		11.020			40.24	
	MOTA	675			A 256					40.24	
	MOTA	676	CA	SER	A 256	-1.883	10.527	53.382	1.00	40.92	С

-142-

	ATOM	677	С	SER A	A 256	-2.148	12.010	53.152	1.00 40.23	С
	ATOM	678	0	SER A	A 256	-1.662	12.599	52.185	1.00 40.28	0
	ATOM	679	CB	SER A	A 256	-2.968	9.693	52.690	1.00 41.53	C
	ATOM	680	OG	SER A	A 256	-4.263	10.203	52.957	1.00 43.52	0
5	ATOM	681	N		A 257	-2.916	12.610	54.056	1.00 39.55	N
	ATOM	682	CA		A 257	-3.252	14.024	53.963	1.00 38.71	C
	ATOM	683	C		A 257	-1.999	14.889	54.038	1.00 36.50	Č
	ATOM	684	ŏ		A 257	-1.825	15.810	53.240	1.00 36.20	ŏ
	ATOM	685	СВ		A 257	-4.221	14.400	55.085	1.00 41.43	Č
10	ATOM	686	CG		A 257	-4.650	15.853	55.090	1.00 44.63	Ċ
••	ATOM	687	CD		A 257	-5.747	16.121	56.103	1.00 47.39	C
	ATOM	688	OE1		A 257	-6.879	15.634	55.896	1.00 48.76	Ö
	ATOM	689	OE2		A 257	-5.476	16.810	57.109	1.00 48.99	0
	MOTA	690	N		A 258	-1.132	14.593	55.001		
15									1.00 34.59	N
13	MOTA	691	CA		A 258	0.111	15.339	55.159	1.00 33.04	C
	MOTA	692	C		A 258	1.064	15.047	54.002	1.00 32.48	C
	ATOM	693	0		A 258	1.782	15.934	53.546	1.00 31.37	0
	ATOM	694	CB		A 258	0.784	14.984	56.488	1.00 34.07	C
00	MOTA	695	CG		A 258	0.256	15.809	57.645	1.00 35.11	C
20	MOTA	696			A 258	0.599	15.501	58.807	1.00 35.63	0
	MOTA	697			A 258	-0.493	16.775	57.386	1.00 34.86	0
	MOTA	698	N		A 259	1.072	13.803	53.532	1.00 31.90	N
	ATOM	699	CA		A 259	1.940	13.433	52.417	1.00 32.81	C
	MOTA	700	C	GLN	A 259	1.611	14.272	51.184	1.00 32.59	C
25	ATOM	701	0		A 259	2.505	14.820	50.534	1.00 32.51	0
	MOTA	702	CB	GLN	A 259	1.783	11.946	52.077	1.00 32.98	C
	MOTA	703	CG	GLN	A 259	2.217	11.000	53.181	1.00 34.94	C
	ATOM	704	CD	GLN	A 259	2.168	9.547	52.755	1.00 37.19	С
	ATOM	705	OE1	GLN	A 259	2.322	8.641	53.576	1.00 39.55	0
30	MOTA	706	NE2	GLN	A 259	1.958	9.315	51.466	1.00 37.81	N
	MOTA	707	N	ILE	A 260	0.325	14.375	50.866	1.00 32.68	N
	MOTA	708	CA	ILE	A 260	-0.109	15.147	49.706	1.00 32.42	C
	MOTA	709	С		A 260	0.183	16.634	49.880	1.00 31.57	C
	ATOM	710	0		A 260	0.588	17.311	48.933	1.00 30.43	Ō
35	ATOM	711	СВ		A 260	-1.619	14.959	49.445	1.00 33.97	Č
	ATOM	712	CG1		A 260	-1.933	13.471	49.277	1.00 34.59	c
	MOTA	713	CG2		A 260	-2.036	15.731	48.201	1.00 33.83	Č
	MOTA	714			A 260	-1.156	12.789	48.165	1.00 36.85	č
	MOTA	715	N		A 261	-0.029	17.146	51.088	1.00 29.87	N
40	ATOM	716	CA		A 261	0.244	18.551	51.358	1.00 28.91	C
. •	ATOM	717	C		A 261	1.717	18.862	51.097	1.00 27.91	Č
	ATOM	718	Ö		A 261	2.043	19.856		1.00 28.13	
	ATOM	719	СВ		A 261	-0.089	18.923	52.827	1.00 28.91	Č
	ATOM	720			A 261	0.472	20.294	53.161	1.00 30.09	
45	ATOM	721			A 261	-1.594	18.911	53.035	1.00 31.46	
••	ATOM	722	N		A 262	2.605	18.011	51.604	1.00 31.40	
	ATOM	723	CA		A 262	4.039	18.222	51.423	1.00 27.17	C
		724	C		A 262	4.461	18.126	49.955	1.00 25.46	
	MOTA	725	Ö		A 262	5.274	18.921	49.485		
50	MOTA								1.00 24.78	
30	ATOM	726	CB		A 262	4.836	17.219	52.265	1.00 26.02	
	MOTA	727	CG		A 262	4.604		53.781	1.00 25.71	
	MOTA	728			A 262	5.382		54.464	1.00 26.98	
	MOTA	729			A 262	5.028		54.317	1.00 26.30	
6E	ATOM	730	N		A 263	3.911		49.232	1.00 25.71	
55	ATOM	731	CA		A 263			47.818	1.00 26.15	
	ATOM	732	C		A 263			46.974	1.00 26.42	
	MOTA	733	0		A 263			46.154	1.00 25.91	
	ATOM	734	CB	LEU	A 263	3.633	15.681	47.283	1.00 27.20	C

-143-

	ATOM	735	CG	LEU A 263	4.293	14.376	47.745	1.00 2	9.34	С
	ATOM	736	CD1	LEU A 263	3.401	13.197	47.404	1.00 3	0.14	C
	MOTA	737	CD2	LEU A 263	5.658	14.223	47.082	1.00 3	1.00	C
	MOTA	738	N	LYS A 264	2.519	18.585	47.178	1.00 2	5.69	N
5	ATOM	739	CA	LYS A 264	1.987	19.699	46.405	1.00 2		C
	MOTA	740	C	LYS A 264	2.709	21.011	46.655	1.00 2	6.97	C
	ATOM	741	0	LYS A 264	2.962	21.767	45.723	1.00 2	7.99	0
	MOTA	742	CB	LYS A 264	0.496	19.899	46.688	1.00 2	9.36	C
	ATOM	743	CG	LYS A 264	-0.417	18.910	45.994	1.00 3	1.84	C
10	ATOM	744	CD	LYS A 264	-1.862	19.348	46.156	1.00 3	35.05	C
	ATOM	745	CE	LYS A 264	-2.822	18.400	45.468	1.00 3	37.95	C
	MOTA	746	NZ	LYS A 264	-4.233	18.872	45.629	1.00 3	39.41	N
	MOTA	747	N	SER A 265	3.047	21.286	47.908	1.00 2	26.64	N
	ATOM	748	CA	SER A 265	3.712	22.540	48.227	1.00 2	27.75	C
15	ATOM	749	С	SER A 265		22.591	47.884	1.00 2	26.92	C
	ATOM	750	0	SER A 265		23.676	47.723	1.00 2	28.28	0
	ATOM	751	СВ	SER A 265		22.881	49.709	1.00 2		C
	ATOM	752	OG	SER A 265		21.902	50.540	1.00 3	33.64	0
	ATOM	753	N	SER A 266		21.434	47.757	1.00 2		N
20	ATOM	754	CA	SER A 266		21.412	47.449	1.00 2		C
	ATOM	755	C	SER A 266		21.035	46.011	1.00		Č
	ATOM	756	ō	SER A 266		21.206	45.572	1.00		ō
	MOTA	757	СВ	SER A 266		20.445	48.385	1.00		Č
	MOTA	758	OG	SER A 266		19.101	48.094	1.00		ō
25	ATOM	759	N	ALA A 267		20.519	45.285	1.00		N
	ATOM	760	CA	ALA A 267		20.089	43.898	1.00		c
	ATOM	761	C	ALA A 267		20.979	43.040	1.00		Ċ
	ATOM	762	ŏ	ALA A 267		20.517	42.515	1.00		ō
	ATOM	763	СВ	ALA A 267		19.938	43.217	1.00		č
30	ATOM	764	N	ILE A 268		22.247	42.883	1.00		N
00	ATOM	765	CA	ILE A 268		23.135	42.041	1.00		c
	ATOM	766	C	ILE A 268		23.374	42.592	1.00		č
	ATOM	767	ŏ	ILE A 268		23.558	41.828		20.90	ŏ
	ATOM	768	CB	ILE A 268		24.496	41.811		23.63	č
35	MOTA	769	CG1			25.232	40.645		24.85	c
00	ATOM	770	CG2			25.252	43.068		25.18	C
	ATOM	771	CD1			24.549	39.303		25.69	Č
	ATOM	772	N	GLU A 26			43.911		20.40	N
	ATOM	773	CA	GLU A 26		23.561	44.529		20.63	C
40	ATOM	774	C	GLU A 26		22.402	44.268		21.33	Č
70	ATOM	775	Ö	GLU A 26		22.620	43.976		20.99	o
	ATOM	776	CB				46.030		20.38	C
				GLU A 26			46.396		22.10	C
	ATOM	777 778	CG CD	GLU A 26			47.892		23.72	c
45	MOTA						48.656		22.73	Ö
70	MOTA	779		L GLU A 26			48.301		24.58	o
	MOTA	780		2 GLU A 26 VAL A 27			44.375		20.39	N
	MOTA	781	N CA	VAL A 27			44.143		20.83	C
	MOTA	782		VAL A 27			42.670		20.53	C
50	MOTA	783		VAL A 27			42.318		20.32	0
30	MOTA	784								
	MOTA	785					44.597 44.318		21.55 21.95	C
	ATOM	786		1 VAL A 27						C
	ATOM	787		2 VAL A 27			46.086		23.25	C
E 5	MOTA	788		ILE A 27					20.29	N
55	MOTA	789							20.71	C
	ATOM	790		ILE A 27					20.86	C
	ATOM	791		ILE A 27					20.78	
	ATOM	792	СВ	ILE A 27	1 10.755	20.684	39.563	1.00	21.89	С

-144-

	MOTA	793		ILE A			9.842	19.450	39.483	-	24.21	C
	ATOM	794	CG2	ILE A			11.149	21.173	38.170		23.03	C
	MOTA	795	CD1	ILE A			8.489	19.711	38.852		27.85	C
_	ATOM	796	N	MET A			13.076	22.481	40.701		21.17	N
5	ATOM	797	CA	MET A			14.147	23.446	40.500	1.00	21.57	C
	ATOM	798	C	MET A			15.474	22.888	41.020	1.00	20.82	C
	MOTA	799	0	MET A	A 2	72	16.513	23.064	40.384	1.00	22.20	0
	MOTA	800	CB	MET A	A 2	72	13.800	24.770	41.183	1.00	22.31	C
	MOTA	801	CG	MET A	A 2'	72	12.595	25.441	40.549	1.00	24.16	C
10	ATOM	802	SD	MET 2	A 2'	72	12.222	27.036	41.296	1.00	26.22	S
	MOTA	803	CE	MET A	A 2'	72	11.003	27.687	40.134	1.00	26.38	C
	ATOM	804	N	LEU A	A 2'	73	15.442	22.204	42.163	1.00	21.17	N
	ATOM	805	CA	LEU 2	A 2	73	16.661	21.606	42.717	1.00	21.28	C
	ATOM	806	С	LEU 2	A 2	73	17.226	20.486	41.842	1.00	20.96	C
15	MOTA	807	0	LEU A	A 2	73	18.408	20.494	41.487	1.00	20.75	0
	MOTA	808	СВ	LEU .			16.405	21.026	44.116		22.98	C
	MOTA	809	CG	LEU .			16.367	21.940	45.337		25.62	C
	ATOM	810	CD1				15.959	21.129	46.572		25.83	C
	ATOM	811	CD2	LEU			17.736	22.571	45.543		26.65	Č
20	ATOM	812	N	ARG			16.385	19.517	41.494		19.69	N
	ATOM	813	CA	ARG			16.852	18.384	40.702		19.52	C
	ATOM	814	C	ARG			17.317	18.787	39.309		19.10	Ċ
	ATOM	815	ŏ	ARG			18.159	18.117	38.715		19.83	ō
	ATOM	816	СВ	ARG			15.759	17.299	40.610		19.75	č
25	ATOM	817	CG	ARG			14.652	17.566	39.601		19.52	č
	ATOM	818	CD	ARG			13.381	16.792	39.969		19.72	Ċ
	ATOM	819	NE	ARG			13.599	15.356	40.153	1.00		N
	ATOM	820	CZ	ARG			13.580	14.453	39.175		19.01	C
	MOTA	821	NH1				13.357	14.824	37.919		18.53	N
30	ATOM	822	NH2	ARG			13.759	13.168	39.458		19.51	N
00	ATOM	823	N	SER			16.792	19.892	38.793		19.73	N
	ATOM	824	CA	SER			17.183	20.331	37.463		19.93	c
	ATOM	825	C	SER			18.615	20.838	37.442	1.00		C
	ATOM	826	Ö	SER			19.191	21.016	36.377		20.21	Ö
35	ATOM	827	СВ	SER			16.249	21.437	36.958		20.51	Č
00	ATOM	828	OG	SER			16.520	22.680	37.579	1.00		0
	ATOM	829	N	ASN			19.198	21.055	38.615	1.00		N
	MOTA	830	CA	ASN			20.564	21.557		1.00		C
	ATOM		-	ASN				20.544	38.662 38.024	1.00		
40		831	C	ASN			21.512 22.585					C
70	MOTA	832	O CB	•				20.903	37.538	1.00		0
	ATOM ATOM	833 834	CG	ASN ASN			20.983	21.843	40.108		20.77	C
												_
	ATOM	835		ASN			23.275	22.187	40.713		26.18	0
15	ATOM	836		ASN			22.231	23.867	39.649		21.92	N
45	MOTA	837	N	GLU			21.096	19.280	38.000		20.52	N
	ATOM	838	CA	GLU			21.925	18.226	37.425		21.75	C
	MOTA	839	C	GLU			22.103	18.370	35.908		21.79	C
	ATOM	840	0	GLU			23.105	17.910	35.351		22.41	0
E 0	ATOM	841	CB	GLU			21.331	16.852	37.785		22.91	C
50	ATOM	842	CG	GLU			22.199	15.659	37.413		26.24	C
	MOTA	843	CD	GLU			21.904	14.418	38.261		28.07	С
	ATOM	844	OE1				22.359	13.319	37.875		30.43	0
	MOTA	845	OE2				21.233	14.532	39.317		26.56	0
	MOTA	846	N	SER			21.152	19.011	35.234		19.68	
55	MOTA	847	CA	SER			21.266	19.194			20.64	
	MOTA	848	С	SER			21.712	20.607	33.448	1.00	21.58	С
	ATOM	849	0	SER	A :	278	22.008	20.910	32.292	1.00	22.05	
	MOTA	850	CB	SER			19.934	18.910	33.092	1.00	20.93	

-145-

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	ATOM	851	OG	SER A			18.941	19.829	33.497		22.00	0
	ATOM	852	N	PHE A	A 2	279	21.751	21.474	34.451	1.00	21.92	N
	ATOM	853	CA	PHE A	A 2	279	22.160	22.853	34.219	1.00	23.24	C
	ATOM	854	C	PHE A	A 2	279	23.659	22.912	33.972	1.00	24.55	C
5	ATOM	855	0	PHE A	A 2	279	24.429	22.218	34.638	1.00	24.49	0
	ATOM	856	CB	PHE 2			21.820	23.723	35.429		23.08	C
	ATOM	857	CG	PHE A			22.051	25.187	35.198		24.02	Č
	ATOM	858	CD1	PHE A			21.135	25.942	34.471		24.96	Ċ
	ATOM	859		PHE			23.197	25.805	35.682		24.94	c
10	ATOM	860	CE1	PHE			21.356	27.293	34.227		24.93	
10	MOTA	861	CE2	PHE A								C
							23.429	27.160	35.442		25.50	C
	MOTA	862	CZ	PHE A			22.506	27.903	34.714		24.47	C
	MOTA	863	N	THR			24.077	23.728	33.010		24.73	N
46	ATOM	864	CA	THR .			25.496	23.872	32.728		26.87	C
15	MOTA	865	С	THR .			25.884	25.343	32.672		27.44	C
	MOTA	866	0	THR .			25.186	26.162	32.070	1.00	26.28	0
	MOTA	867	CB	THR .			25.897	23.198	31.399	1.00	27.76	C
	MOTA	868	OG1	THR .	A 2	280	27.298	23.408	31.173	1.00	31.72	O
	ATOM	869	CG2	THR	A 2	280	25.107	23.768	30.236	1.00	27.79	C
20	ATOM	870	N	MET	A :	281	26.991	25.676	33.326		28.33	N
	MOTA	871	CA	MET			27.469	27.049	33.340		31.03	C
	ATOM	872	C	MET			28.275	27.390	32.095		31.28	Č
	ATOM	873	Ö	MET			28.812	28.490	31.980		30.87	ŏ
	MOTA	874	СВ	MET			28.298	27.306	34.596		33.43	Č
25	ATOM	875	CG	MET			27.448	27.518	35.835		36.11	Č
	ATOM	876	SD	MET			28.429	27.829	37.295		39.85	s
	ATOM	877	CE									
				MET			28.995	29.495	36.967		40.40	С
	ATOM	878	N	ASP			28.364	26.448	31.159		31.72	N
20	ATOM	879	CA	ASP			29.097	26.709	29.925		32.91	С
30	MOTA	880	С	ASP			28.366	27.818	29.175		32.02	C
	MOTA	881	0	ASP			28.989	28.764	28.683		31.15	0
	ATOM	882	CB	ASP			29.172	25.455	29.050	1.00	35.93	C
	MOTA	883	CG	ASP	Α	282	29.947	24.328	29.708	1.00	39.91	C
	ATOM	884	OD1	ASP	Α	282	30.940	24.619	30.412	1.00	42.35	0
35	ATOM	885	OD2	ASP	A	282	29.573	23.150	29.508	1.00	42.45	0
	ATOM	886	N	ASP	Α	283	27.041	27.702	29.100	1.00	29.87	N
	MOTA	887	CA	ASP	Α	283	26.224	28.704	28.418	1.00	28.59	С
	ATOM	888	С	ASP	Α	283	24.931	29.032	29.170	1.00	27.92	C
	ATOM	889	0	ASP			23.984	29.568	28.592		27.21	ō
40	ATOM	890	СВ	ASP			25.904	28.243	26.994		29.84	Č
	ATOM	891	CG	ASP			25.030	27.006	26.958		31.11	Č
	ATOM	892		ASP		283	24.872	26.351	28.009		28.99	Ö
	ATOM	893		ASP			24.507	26.687	25.870		32.79	ŏ
	ATOM	894	N N	MET			24.902	28.708	30.460		26.84	
45												N
73	ATOM	895	CA	MET			23.748	28.985	31.317		27.62	C
	ATOM	896	C	MET			22.449	28.379	30.801		27.20	C
	MOTA	897	0	MET			21.429	29.060	30.686		27.86	0
	MOTA	898	CB	MET			23.565	30.497	31.484		29.95	С
	MOTA	899	CG	MET			24.785	31.219	32.031		33.34	С
50	ATOM	900	SD	MET			25.323	30.578	33.624		36.23	S
	ATOM	901	CE	MET			26.985	31.242	33.719		35.78	C
	ATOM	902	N	SER	A	285	22.479	27.091	30.503	1.00	25.58	N
	ATOM	903	CA	SER	Α	285	21.288	26.427	30.010	1.00	24.62	С
	ATOM	904	С	SER	A	285	21.136	25.090	30.697		24.72	C
55	MOTA	905	0			285	22.028	24.641	31.415		24.18	ō
	MOTA	906	СB			285	21.402	26.186	28.509		24.98	c
	ATOM	907	OG			285	22.415	25.224	28.241		25.94	Ö
	ATOM	908	N			286	19.982	24.472	30.480			
	NION.	200	7.4	IKP	^	200	13.302	44.412	30.400	1.00	24.17	N

-146-

	B TOM	909	CA	mpp 1		206	10 600	22 146	30 007	1 00	04 74	_
	MOTA			TRP A			19.699	23.146	30.997		24.74	C
	MOTA	910		TRP A			19.842	22.312	29.732		25.34	C
	ATOM	911		TRP A			19.006	22.391	28.828		25.37	0
E	ATOM	912		TRP A			18.268	23.064	31.522		23.76	C
5	MOTA	913		TRP A			18.048	23.702	32.863		21.76	C
	MOTA	914		TRP A			18.186	23.107	34.088		21.47	C
	MOTA	915		TRP A			17.568	25.031	33.118		23.03	C
	MOTA	916	NE1	TRP A	A :	286	17.811	23.976	35.084	1.00	21.88	N
	MOTA	917	CE2	TRP A	A :	286	17.429	25.164	34.519	1.00	22.96	C
10	ATOM	918	CE3	TRP A	A :	286	17.238	26.121	32.299	1.00	23.54	C
	MOTA	919	CZ2	TRP 2	A :	286	16.970	26.341	35.120	1.00	24.15	C
	ATOM	920	CZ3	TRP 2	A	286	16.781	27.293	32.898	1.00	22.92	C
	ATOM	921	CH2	TRP 2	A	286	16.651	27.390	34.297		23.66	C
	ATOM	922	N	THR			20.918	21.540	29.654		25.53	N
15	MOTA	923	CA	THR			21.173	20.721	28.478		27.14	C
• •	ATOM	924	C	THR			20.833	19.266	28.753		27.53	Č
	ATOM	925	ō	THR			21.501	18.607	29.551	1.00		ŏ
	ATOM	926	СВ	THR			22.644	20.853	28.049		27.77	Č
	ATOM	927	OG1	THR			22.914	22.229				
20			CG2						27.733		30.32	0
20	ATOM	928		THR .			22.922	20.000	26.824		29.69	C
	ATOM	929	N	CYS			19.792	18.775	28.084		28.08	N
	ATOM	930	CA	CYS			19.326	17.406	28.270		30.34	С
	ATOM	931	С	CYS			19.478	16.520	27.040		33.66	C
05	MOTA	932	0	CYS			18.530	15.857	26.624		33.19	0
25	MOTA	933	CB	CYS			17.861	17.426	28.699	1.00	29.32	C
	MOTA	934	SG	CYS			17.566	18.403	30.188	1.00	28.01	S
	ATOM	935	N	GLY	A	289	20.675	16.498	26.466	1.00	37.69	N
	MOTA	936	CA	GLY	Α	289	20.897	15.682	25.286	1.00	41.85	C
	MOTA	937	C	GLY	Α	289	21.072	16.536	24.044	1.00	44.11	C
30	ATOM	938	0	GLY	Α	289	21.842	17.497	24.051	1.00	45.10	0
	MOTA	939	N	ASN	Α	290	20.349	16.205	22.978		46.33	N
	ATOM	940	CA	ASN			20.469	16.959	21.737		47.32	C
	ATOM	941	C	ASN			19.961	18.391	21.874		47.22	Ċ
	ATOM	942	Ö	ASN			19.303	18.746	22.857		47.49	ō
35	ATOM	943	СВ	ASN			19.733	16.241	20.600		49.56	Č
	ATOM	944	CG	ASN			18.235	16.224	20.792		51.07	č
	ATOM	945	OD1	ASN			17.591	17.271	20.792	1.00		Ö
	ATOM	946	ND2				17.668	15.032	20.944	1.00		
		947	ND2	GLN			20.277					N
40	ATOM							19.205	20.874	1.00		N
40	ATOM	948	CA	GLN			19.896	20.611	20.850		45.60	C
	ATOM	949	C	GLN			18.402	20.859	21.031		43.20	C
	MOTA	950	0	GLN			18.007	21.916	21.520		43.27	0
	ATOM	951	CB	GLN			20.380	21.247	19.545		47.46	C
AE	ATOM	952	CG			291	21.879	21.087	19.325		50.94	C
45	ATOM	953	CD			291	22.705	21.786	20.395		52.59	C
	ATOM	954		GLN			23.893	21.503	20.563		54.12	0
	ATOM	955	NE2	GLN			22.081	22.712	21.114		53.69	N
	MOTA	956	N	ASP	Α	292	17.574	19.897	20.636	1.00	40.92	N
	MOTA	957	CA	ASP	Α	292	16.129	20.046	20.780	1.00	38.58	C
50	ATOM	958	С	ASP	Α	292	15.740	20.140	22.252	1.00	35.80	C
	ATOM	959	0	ASP	A	292	14.769	20.814	22.601	1.00	34.04	0
	ATOM	960	CB	ASP	Α	292	15.391	18.862	20.145	1.00	41.69	С
	ATOM	961	CG			292	15.325	18.950	18.629		44.13	C
	ATOM	962		ASP			14.862	17.973	18.002		45.48	ō
55	ATOM	963		ASP				19.993	18.067		45.78	ŏ
_	ATOM	964	N			293		19.469	23.111		33.09	N
	ATOM	965	CA			293		19.465	24.543		31.43	c
	ATOM	966	C			293		20.305	25.367		30.28	C
	011	200	-	\				20.303	23.307	1.00	. 50.40	C

-147-

	ATOM	967	0	TYR A	. 2	93	17.558	19.934	26.481	1.00	30.56	0
	MOTA	968	CB	TYR A	. 2	93	16.186	18.027	25.066	1.00	31.64	C
	MOTA	969	CG	TYR A	\ 2	93	15.232	17.154	24.287	1.00	31.43	C
_	ATOM	970		TYR A			15.591	15.864	23.905		32.22	C
5	ATOM	971		TYR A			13.999	17.647	23.861		32.09	C
	MOTA	972	CE1	TYR A	1 2	293	14.752	15.091	23.106	1.00	32.84	C
	MOTA	973	CE2	TYR A	1 2	293	13.153	16.883	23.063		31.78	C
	MOTA	974	CZ	TYR A			13.537	15.611	22.684		33.14	C
	ATOM	975	OH	TYR A			12.726	14.874	21.850		32.75	0
10	MOTA	976	N	LYS A			17.594	21.431	24.801		29.44	N
	MOTA	977	CA	LYS A			18.466	22.369	25.494		27.92	C
	MOTA	978	C	LYS A			17.529	23.530	25.786		27.57	C
	ATOM	979	0	LYS A			16.947	24.114	24.866		27.85	0
	MOTA	980	CB	LYS A			19.618	22.833	24.595		31.41	C
15	MOTA	981	CG	LYS A			20.500	23.907	25.239		32.77	C
	ATOM	982	CD	LYS A			21.578	24.416	24.284	1.00		C
	MOTA	983	CE	LYS A			22.872	23.633	24.419		37.32	C
	MOTA	984	NZ	LYS 2			23.599	23.990	25.673		37.49	N
	MOTA	985	N	TYR 2			17.363	23.852	27.061		25.07	N
20	ATOM	986	CA	TYR A			16.465	24.928	27.451		24.97	C
	MOTA	987	C	TYR			17.208	26.154	27.938		25.69	C
	ATOM	988	0	TYR .			18.005	26.074	28.865		24.37	0
	MOTA	989	CB	TYR .			15.517	24.431	28.543		24.19	C
	ATOM	990	CG	TYR .			14.927	23.080	28.216		24.03	C
25	MOTA	991	CD1				15.297	21.943	28.932		23.33	C
	MOTA	992		TYR			14.023	22.933	27.167		23.84	C
	MOTA	993	CE1				14.780	20.692	28.611		24.85	C
	MOTA	994	CE2				13.500	21.688	26.836		24.18	С
	MOTA	995	CZ	TYR			13.882	20.573	27.563		24.74	C
30	MOTA	996	OH	TYR			13.369	19.338	27.244		24.72	0
	MOTA	997	N	ARG			16.921	27.286	27.302		27.37	N
	MOTA	998	CA	ARG			17.532	28.566	27.632		29.21	C
	MOTA	999	С	ARG			16.457	29.505	28.177		28.74	С
0.5	ATOM	1000	0	ARG			15.269	29.177	28.171	1.00		0
35	ATOM	1001	CB	ARG			18.140	29.201	26.377	1.00		C
	MOTA	1002	CG	ARG			19.115	28.332	25.590	1.00		С
	ATOM	1003	CD	ARG			19.581	29.091	24.352		40.42	С
	MOTA	1004	NE	ARG			20.676	28.444	23.631		44.23	N
40	MOTA	1005	CZ	ARG			20.533	27.442	22.769		46.02	С
40	ATOM	1006		ARG			19.329	26.949	22.508		46.77	N
	ATOM	1007		ARG			21.597	26.941	22.152		46.52	N
	MOTA	1008	N	VAL			16.879	30.678	28.634		29.11	N
	ATOM	1009	CA	VAL			15.956	31.675	29.167		30.41	C
AE	ATOM	1010	C	VAL			14.821	31.972	28.187		30.24	C
45	MOTA	1011	0	VAL			13.655	32.065	28.582		29.94	0
	MOTA	1012	CB	VAL			16.692	33.005	29.475		30.71	C
	MOTA	1013		VAL			15.686	34.103	29.797		33.35	C
	MOTA	1014		VAL			17.646	32.811	30.644		32.09	
5 0	MOTA	1015	N			298	15.168	32.115	26.912		30.44	
50	MOTA	1016	CA			298	14.185	32.430	25.881		30.65	
	ATOM	1017	С			298	13.106	31.370	25.714		30.99	
	MOTA	1018	0			298	11.986	31.680	25.304		31.34	
	MOTA	1019	CB			298		32.675	24.539		31.86	
EE	ATOM	1020	OG			298	15.658	31.559			33.35	
55	ATOM	1021	N			299					29.88	
	ATOM	1022				299					29.41	
	ATOM	1023				299					28.20	
	MOTA	1024	0	ASP	Α	299	10.268	28.770	26.827	1.00	28.75	0

-148-

	ATOM	1025	СВ	ASP A	299	13.162	27.679	25.979	1.00	31.09	С
	MOTA	1026	CG	ASP A	299	14.070	27.435	24.797	1.00	34.22	C
	MOTA	1027	OD1	ASP A	299	13.589	27.548	23.651	1.00	34.74	0
_	MOTA	1028	OD2	ASP A		15.263	27.129	25.013	1.00	36.25	0
5	MOTA	1029	N	VAL A	300	11.837	29.631	28.183	1.00		N
	MOTA	1030	CA	VAL A	300	10.923	29.760	29.308	1.00	26.53	C
	MOTA	1031	С	VAL A	A 300	9.948	30.913	29.070	1.00	26.97	C
	MOTA	1032	0	VAL A	A 300	8.781	30.835	29.449	1.00	26.32	0
	MOTA	1033	CB	VAL A		11.703	29.972	30.623	1.00	27.74	C
10	ATOM	1034	CG1	VAL A	A 300	10.749	29.958	31.811	1.00	29.57	C
	MOTA	1035	CG2	VAL A	A 300	12.757	28.871	30.772	1.00		C
	MOTA	1036	N	THR A		10.420	31.980	28.432	1.00	26.55	N
	MOTA	1037	CA		A 301	9.539	33.106	28.142	1.00	27.35	C
	MOTA	1038	C	THR A	A 301	8.507	32.672	27.100	1.00		C
15	MOTA	1039	0	THR A	A 301	7.394	33.188	27.069	1.00	27.90	0
	ATOM	1040	CB	THR A	A 301	10.324	34.329	27.617	1.00	27.90	C
	ATOM	1041	OG1		A 301	11.097	33.956	26.472	1.00	29.74	0
	MOTA	1042	CG2	THR A		11.250	34.861	28.696	1.00	29.44	C
	ATOM	1043	N		A 302	8.875	31.715	26.250	1.00	26.49	N
20	MOTA	1044	CA	LYS 2	A 302	7.948	31.225	25.232	1.00	27.28	C
	MOTA	1045	С		A 302	6.886	30.318	25.847	1.00	27.81	C
	MOTA	1046	0		A 302	5.960	29.874	25.160	1.00	27.95	0
	MOTA	1047	CB	LYS	A 302	8.701	30.477	24.130	1.00	28.36	C
	MOTA	1048	CG	LYS .	A 302	9.496	31.386	23.206	1.00	29.79	C
25	MOTA	1049	CD	LYS .	A 302	10.203	30.586	22.128	1.00	30.72	C
	MOTA	1050	CE		A 302	11.019	31.482	21.209		32.93	С
	MOTA	1051	NZ		A 302	12.121	32.161	21.934	1.00	33.88	N
	MOTA	1052	N		A 303	7.019	30.048	27.143		26.44	N
	MOTA	1053	CA		A 303	6.052	29.219	27.847			С
30	MOTA	1054	C		A 303	5.130	30.097	28.692		28.91	С
	MOTA	1055	0		A 303	4.310	29.592	29.457		29.81	0
	MOTA	1056	CB		A 303	6.771	28.199	28.726		27.38	C
	MOTA	1057	N		A 304	5.279	31.415	28.564		29.66	N
0.5	MOTA	1058	CA		A 304	4.423	32.328	29.309		30.57	C
35	MOTA	1059	C		A 304	4.963	32.961	30.582		31.32	C
	MOTA	1060	0		A 304	4.257	33.735	31.234		32.07	0
	ATOM	1061	N		A 305	6.202	32.649	30.948		31.10	N
	ATOM	1062	CA		A 305	6.797	33.216	32.155		30.95	С
40	MOTA	1063	С	HIS		7.656	34.439	31.853		31.77	C
40	ATOM	1064	0	HIS		8.138	34.610	30.731		31.65	0
	MOTA	1065	CB		A 305	7.628	32.155	32.881		30.92	С
	MOTA	1066	CG	HIS		6.799	31.128	33.585		30.70	С
	ATOM	1067			A 305	6.017	31.430	34.679		31.24	N
AE	MOTA	1068			A 305	6.599	29.812	33.331		31.47	C
45	ATOM	1069			A 305	5.369	30.346	35.067		31.89	C
	MOTA	1070			A 305	5.704	29.351	34.265		30.48	N
	MOTA	1071	N		A 306	7.839	35.290	32.860		32.01	N
	ATOM	1072	CA		A 306	8.624	36.511	32.700		33.97	C
5 0	ATOM	1073	C		A 306	9.982	36.449	33.392		34.00	C
50	ATOM	1074	0		A 306	10.265	35.523	34.154		33.09	0
	ATOM	1075	CB		A 306	7.842	37.710	33.235		34.42	C
	ATOM	1076	OG		A 306	7.739	37.654	34.645		37.62	0
	ATOM	1077	N		A 307	10.813	37.455	33.125		34.07	N
55	MOTA	1078	CA		A 307	12.155	37.537	33.694		34.93	C
J J	ATOM	1079	C		A 307	12.172	37.666	35.212		33.80	C
	MOTA	1080	0		A 307	13.180	37.364	35.851		33.69	0
	MOTA	1081	CB		A 307	12.923	38.710	33.068		36.84	C
	MOTA	1082	CG	LEU	A 307	13.434	38.527	31.634	1.00	39.29	C

-149-

	MOTA	1083		LEU A		12.282	38.235	30.685	1.00 4		C
	MOTA	1084	CD2	LEU A	307	14.168	39.784	31.201	1.00 4		C
	MOTA	1085	N	GLU A	308	11.060	38.110	35.789	1.00 3		N
_	MOTA	1086		GLU A		10.963	38.265	37.235	1.00 3	2.81	C
5	MOTA	1087	С	GLU A	308		36.913	37.917	1.00 3		C
	MOTA	1088	0	GLU A	308	11.558	36.842	39.078	1.00 3	30.22	0
	ATOM	1089	CB	GLU A	308	9.603	38.856	37.607	1.00 3		C
	MOTA	1090	CG	GLU A	308	9.308	40.169	36.888	1.00 4	12.70	C
	ATOM	1091	CD	GLU A	308	7.914	40.707	37.166	1.00 4	15.49	C
10	ATOM	1092	OE1	GLU A	A 308	7.522	41.696	36.507	1.00 4	16.94	0
	ATOM	1093	OE2	GLU A	308	7.214	40.149	38.040	1.00 4	17.58	0
	MOTA	1094	N	LEU A	A 309	10.898	35.838	37.182	1.00 2	29.69	N
	ATOM	1095	CA	LEU A	A 309	11.081	34.492	37.714	1.00 2	29.34	C
	ATOM	1096	С	LEU Z	A 309		33.872	37.130	1.00 2	28.31	C
15	ATOM	1097	0	LEU Z			33.290	37.848	1.00 2		0
	ATOM	1098	СВ	LEU Z			33.605	37.360	1.00 2		C
	ATOM	1099	CG	LEU 2			32.116	37.700	1.00 2		С
	ATOM	1100		LEU			31.931	39.211	1.00		Ċ
	ATOM	1101		LEU			31.312	37.048	1.00		C
20	ATOM	1102	N		A 310		34.019	35.822	1.00		N
	ATOM	1103	CA		A 310		33.428	35.142	1.00		c
	MOTA	1104	C		A 310		33.907	35.590	1.00		Ċ
	ATOM	1105	ŏ		A 310		33.092	35.808	1.00		Ö
	ATOM	1106	СВ		A 310		33.605	33.617	1.00		Č
25	ATOM	1107	CG1		A 310		33.023	33.139	1.00		č
20	ATOM	1108	CG2		A 310		32.884	32.918	1.00		č
	ATOM	1100	CD1		A 31		33.289	31.681	1.00		č
	ATOM	1110	N		A 31		35.213	35.726		31.83	N
	ATOM	1111	CA		A 31		35.707	36.151		33.28	C
30	ATOM	1111	C		A 31		35.707	37.528		31.76	c
50	ATOM	1113	o		A 31		34.707	37.714		31.24	Ö
		1114	СВ		A 31		37.237	36.128		35.65	č
	MOTA MOTA	1115	CG		A 31		37.788	34.710		41.13	c
		1116	CD		A 31		39.287	34.710		43.32	C
35	ATOM	1117	OE1		A 31		39.815	33.522		46.68	ŏ
33	MOTA		OE2		A 31		39.933	35.718		45.68	Ö
	MOTA	1118					35.232	38.511		30.94	N
	MOTA	1119	N		A 31 A 31		34.728	39.851		29.89	C
	MOTA	1120	CA				33.212	39.831		28.28	c
40	MOTA	1121	C		A 31		32.656			28.14	Ö
40	ATOM	1122	0		A 31		35.115	40.619 40.675		30.62	C
	MOTA	1123	CB		A 31			39.962		31.93	C
	ATOM	1124	CG		A 31						
	ATOM	1125	CD		A 31		35.943	38.523		31.29	C
45	ATOM	1126	N		A 31			38.883		26.85	N
45	MOTA	1127	CA		A 31		31.102	38.739		26.51	C
	ATOM	1128	C		A 31			38.267		25.16	C
	MOTA	1129	0		A 31			38.788		24.33	0
	ATOM	1130	CB		A 31			37.715		27.97	C
50	ATOM	1131	CG		A 31			37.935		31.36	C
50	MOTA	1132		L LEU				36.600		29.96	C
	MOTA	1133		2 LEU				38.536		30.03	C
	MOTA	1134			A 31			37.279		25.12	
	MOTA	1135			A 31					25.36	
	MOTA	1136			A 31					25.44	
55	MOTA	1137			A 31					25.07	
	MOTA	1138			A 31					26.51	
	MOTA	1139		1 ILE						28.21	
	ATOM	1140	CG	2 ILE	A 3	L4 20.982	31.844	35.028	1.00	26.75	C

-150-

	MOTA	1141	CD1	ILE A	314	18.654	30.407	33.858	1.00		С
	MOTA	1142	N	LYS A	315	20.112	32.641	38.574	1.00	25.44	N
	MOTA	1143	CA	LYS ?	315		32.994	39.626	1.00		C
_	MOTA	1144		LYS A			31.869	40.656	1.00		C
5	MOTA	1145		LYS /			31.522	41.149	1.00		0
	ATOM	1146	CB	LYS A	315	20.651	34.310	40.296	1.00	28.77	C
	MOTA	1147	CG	LYS A	A 315	21.759	34.926	41.134	1.00		C
	MOTA	1148	CD	LYS A			36.427	41.306	1.00		C
	MOTA	1149	CE	LYS A			37.082	41.891		39.12	C
10	MOTA	1150	NZ	LYS A			36.521	43.227		41.56	N
	MOTA	1151	N	PHE A			31.295	40.967		23.92	N
	MOTA	1152	CA	PHE A	A 316	19.874	30.196	41.921		23.22	C
	MOTA	1153	С	PHE 2			28.997	41.400		22.36	C
	MOTA	1154	0	PHE A			28.380	42.151		22.35	0
15	MOTA	1155	CB	PHE .	A 316	5 18.410	29.791	42.144	1.00	24.22	C
	ATOM	1156	ÇG	PHE .	A 316	18.242	28.546	42.979		26.30	C
	ATOM	1157	CD1	PHE .	A 316	5 18.323	28.605	44.370	1.00	27.43	C
	MOTA	1158		PHE .			27.310	42.372	1.00	26.87	C
	MOTA	1159	CE1	PHE .	A 310	6 18.204	27.446	45.141	1.00	28.46	C
20	ATOM	1160	CE2	PHE	A 31	5 17.918	26.145	43.135	1.00	27.51	C
	MOTA	1161	CZ	PHE	A 31	5 18.002	26.218	44.520	1.00	28.27	C
	MOTA	1162	N	GLN	A 31'	7 20.480	28.665	40.120	1.00	21.28	N
	ATOM	1163	CA	GLN	A 31	7 21.175	27.524	39.522	1.00	21.35	C
	MOTA	1164	C	GLN	A 31	7 22.694	27.681	39.586	1.00	21.92	C
25	MOTA	1165	0	GLN	A 31	7 23.410	26.735	39.913	1.00	20.68	0
	ATOM	1166	CB	GLN	A 31	7 20.754	27.324	38.057		21.98	C
	MOTA	1167	CG		A 31		26.891	37.855	1.00	22.78	C
	MOTA	1168	CD	GLN	A 31	7 18.968	25.585	38.563	1.00	25.08	C
	ATOM	1169	OE1	GLN	A 31	7 19.792	24.670	38.619		26.08	0
30	ATOM	1170	NE2	GLN	A 31	7 17.756	25.488	39.093	1.00	22.14	N
	ATOM	1171	N		A 31		28.870	39.259	1.00	22.58	N
	MOTA	1172	CA	VAL	A 31	8 24.629	29.108	39.301	1.00	23.76	C
	MOTA	1173	С	VAL	A 31	8 25.162	28.983	40.734	1.00	24.71	C
	MOTA	1174	0	VAL	A 31	8 26.199	28.349	40.971	1.00	26.38	0
35	MOTA	1175	CB	VAL	A 31	8 24.975	30.510	38.727		24.56	С
	MOTA	1176	CG1	VAL	A 31		30.798	38.897		26.05	C
	MOTA	1177	CG2	VAL			30.567	37.255		23.60	C
	ATOM	1178	N		A 31		29.574	41.687		25.34	N
	ATOM	1179	CA		A 31			43.076		26.42	С
40	MOTA	1180	C		A 31			43.623		26.70	С
	MOTA	1181	0		A 31			44.399		26.15	0
	MOTA	1182	N		A 32			43.226		25.08	N
	ATOM	1183	CA		A 32			43.680		26.49	С
45	MOTA	1184	С		A 32			43.019		26.16	C
45	MOTA	1185	0		A 32			43.666		25.62	0
	MOTA	1186	CB		A 32			43.318		26.17	С
	MOTA	1187	CG		A 32			43.877		29.00	С
	MOTA	1188		. LEU				45.394		28.44	С
50	MOTA	1189		LEU				43.439		27.28	С
50	ATOM	1190	N		A 32			41.734		26.97	N
	MOTA	1191	CA		A 32			41.000		29.33	C
	ATOM	1192	C		A 32			41.649		30.36	C
	ATOM	1193	0		A 32			41.746		30.00	
EE	ATOM	1194	CB		A 32			39.561		30.33	
55	ATOM	1195	CG		A 32					33.36	
	ATOM	1196	CD		A 32					33.34	
	MOTA	1197	CE		A 32					33.36	
	MOTA	1198	NZ	LYS	A 32	21 25.668	20.911	37.111	1.00	32.77	N

-151-

	MOTA	1199	N	LYS A	١.	322	27.894	26.222	42.077	1.00	30.82	N
	ATOM	1200	CA	LYS A	A :	322	29.155	26.601	42.702	1.00	32.19	C
	MOTA	1201	C	LYS !	A :	322	29.447	25.934	44.037	1.00	32.03	C
_	MOTA	1202	0	LYS A	A :	322	30.598	25.896	44.462	1.00	32.87	0
5	MOTA	1203	CB	LYS A	A :	322	29.234	28.122	42.866	1.00	33.78	C
	MOTA	1204		LYS 2			29.592	28.853	41.587	1.00	37.24	C
	MOTA	1205	CD	LYS /	A :	322	29.849	30.328	41.856	1.00	39.61	C
	ATOM	1206	CE	LYS A	Α :	322	30.611	30.964	40.712	1.00	41.25	C
	MOTA	1207	NZ	LYS A	A :	322	31.956	30.335	40.544	1.00	43.80	N
10	MOTA	1208		LEU A			28.420	25.415	44.703	1.00	30.51	N
	MOTA	1209		LEU A			28.627	24.747	45.985	1.00	31.09	C
	MOTA	1210	C	LEU A	A.	323	29.296	23.392	45.774	1.00	31.05	C
	MOTA	1211	0	LEU A	A	323	29.833	22.805	46.715	1.00	31.05	0
	MOTA	1212		LEU 2			27.297	24.544	46.719	1.00	30.29	C
15	ATOM	1213	CG	LEU 2	A	323	26.551	25.784	47.220	1.00	31.62	C
	MOTA	1214	CD1	LEU /	A	323	25.260	25.359	47.904	1.00	30.41	C
	ATOM	1215	CD2	LEU .	A	323	27.434	26.570	48.180	1.00	31.32	C
	MOTA	1216	N	ASN .	A	324	29.264	22.908	44.535	1.00	30.91	N
	MOTA	1217	CA	ASN .			29.854	21.619	44.180	1.00	32.42	C
20	MOTA	1218	C	ASN .			29.466	20.524	45.165	1.00	32.07	C
	MOTA	1219	0	ASN .	A	324	30.323	19.864	45.755	1.00	32.62	0
	MOTA	1220	CB	ASN .	A	324	31.380	21.722	44.110	1.00	36.14	C
	MOTA	1221	CG	ASN	A	324	31.853	22.576	42.954		38.53	C
	MOTA	1222		ASN			32.013	23.789	43.087		43.04	0
25	MOTA	1223	ND2	ASN	A	324	32.068	21.947	41.805	1.00	40.87	N
	MOTA	1224	N	LEU			28.166	20.326	45.333		29.80	N
	MOTA	1225	CA	LEU			27.667	19.320	46.257	1.00	27.98	C
	MOTA	1226	С	LEU			27.969	17.890	45.836		27.42	C
00	MOTA	1227	0	LEU			27.984	17.568	44.648		27.50	0
30	MOTA	1228	CB	LEU			26.149	19.454	46.409		28.15	С
	MOTA	1229	CG	LEU			25.592	20.785	46.907		28.88	C
	MOTA	1230		LEU			24.072	20.701	46.960		29.23	C
	MOTA	1231					26.163	21.105	48.276		28.09	С
05	MOTA	1232	N	HIS			28.219	17.033	46.821		26.59	N
35	MOTA	1233	CA	HIS			28.430	15.618	46.546		25.79	C
	ATOM	1234	C	HIS			27.003	15.162	46.264		25.33	С
	ATOM	1235	0	HIS			26.052	15.819	46.695		23.44	0
	MOTA	1236	CB	HIS			28.935	14.882	47.788		27.17	C
40	ATOM	1237	CG	HIS			30.303	15.294	48.231		27.36	С
40	MOTA	1238		HIS			30.942	14.704	49.301		28.09	N
	ATOM	1239		HIS			31.159	16.222	47.744		28.85	C
	ATOM	1240		HIS					49.453		28.02	
	ATOM	1241		HIS			32.292	16.174	48.521		29.20	N
45	MOTA	1242	N			327		14.054	45.554		24.49	N
45	ATOM	1243	CA			327	25.497	13.569	45.267		24.94	C
	ATOM	1244	C			327	24.768	13.297	46.583		24.29	C
	ATOM	1245	0			327	23.553	13.498	46.686		24.42	0
	MOTA	1246	CB			327		12.302	44.409		27.30	C
50	ATOM	1247	CG			327		11.755	44.032		29.69	
50	ATOM	1248	CD			327		10.740	42.903		32.63	C
	MOTA	1249		GLU				9.771	43.015		31.56	
	ATOM	1250		GLU				10.915	41.903		32.79	
	ATOM	1251	N			328		12.858	47.595		22.79	
55	ATOM	1252	CA			328		12.576	48.911		23.11	
J	ATOM	1253	C			328		13.822	49.500		23.46	
	ATOM	1254	O CB			328		13.750	50.086		23.51	
	ATOM	1255	CB			328		12.083	49.877		24.71	
	MOTA	1256	CG	GLU	A	328	26.540	10.666	49.607	1.00	25.97	С

	ATOM	1257	CD (GLU A	328	27.584	10.591	48.506	1.00 28		C
	MOTA	1258		GLU A		28.201	9.512	48.356	1.00 29		0
	ATOM	1259		GLU A		27.793	11.591	47.789	1.00 27		0
_	MOTA	1260		GLU A		24.939	14.965	49.349	1.00 22		N
5	MOTA	1261		GLU A		24.406	16.221	49.861	1.00 23		C
	MOTA	1262		GLU A			16.678	49.026	1.00 23		C
	ATOM	1263		GLU A		22.236	17.203	49.558	1.00 23		0 C
	MOTA	1264		GLU A			17.281	49.856 50.859	1.00 2		C
10	ATOM	1265		GLU A			16.943 17.599	50.554	1.00 2		C
10	ATOM	1266		GLU A			17.533	51.429	1.00 2		Ö
	ATOM	1267	_	GLU A			18.160	49.454	1.00 2		ŏ
	ATOM	1268 1269		HIS A			16.450	47.721	1.00 2		N
	ATOM ATOM	1270		HIS A			16.836	46.803	1.00 2		C
15	ATOM	1271		HIS A			16.139	47.150	1.00 2		Č
10	ATOM	1272		HIS ?			16.790	47.257	1.00 2		ō
	ATOM	1273		HIS A			16.494	45.364	1.00 2		Ċ
	ATOM	1274	CG	HIS A			16.916	44.321	1.00 2		C
	ATOM	1275		HIS A			18.237	44.060	1.00 2		N
20	ATOM	1276		HIS A			16.190	43.444	1.00 2	5.76	С
	ATOM	1277		HIS A			18.307	43.065	1.00 2	6.73	C
	ATOM	1278		HIS A			17.078	42.674	1.00 2	5.08	N
	ATOM	1279	N	VAL A	A 331	L 20.955	14.823	47.334	1.00 2	2.22	N
	ATOM	1280	CA	VAL .	A 33:	19.739	14.072	47.642	1.00 2	3.00	C
25	MOTA	1281	C	VAL .	A 33:	1 19.185	14.382	49.024	1.00 2		C
	MOTA	1282	0	VAL .	A 33	17.968	14.393	49.218	1.00 2		0
	MOTA	1283	CB	VAL	A 33	1 19.952	12.544	47.490	1.00 2		C
	MOTA	1284	CG1				12.233	46.053	1.00 2		С
	MOTA	1285	CG2	VAL			12.045	48.466	1.00 2		С
30	MOTA	1286	N		A 33		14.634	49.986	1.00 2		N
	MOTA	1287	CA		A 33		14.967	51.327	1.00 2		C
	MOTA	1288	C		A 33		16.311	51.301	1.00		C
	MOTA	1289	0		A 33		16.489	51.976	1.00		0
25	MOTA	1290	CB		A 33		15.020	52.303	1.00 2		C
35	ATOM	1291	CG		A 33		13.656 13.777	52.824 53.516	1.00		c
	MOTA	1292		LEU				53.776	1.00		C
	ATOM	1293			A 33			50.508	1.00		N
	MOTA	1294 1295	N CA		A 33			50.420	1.00		C
40	MOTA	1295	CA		A 33			49.808	1.00		č
40	MOTA MOTA	1297	0		A 33			50.259	1.00		ō
	ATOM	1298	СВ	LEU				49.599	1.00		Č
	ATOM	1299	CG		A 33			49.597	1.00	26.05	C
	ATOM	1300		LEU				51.014	1.00		С
45	ATOM	1301		LEU				48.703	1.00	26.03	С
	ATOM	1302	N		A 33			48.776	1.00	21.27	N
	ATOM	1303	CA		A 33		17.513	48.163		20.93	С
	ATOM	1304	С		A 33		16.881	49.171		21.48	C
	ATOM	1305		MET	A 33	34 13.769	17.263	49.256		21.52	0
50	ATOM	1306	CB	MET	A 33	34 15.939	16.648			21.53	C
	MOTA	1307			A 33					22.31	C
	MOTA	1308	SD		A 33					24.84	
	MOTA	1309			A 3					24.19	
	MOTA	1310			A 3					21.64	
55	MOTA	1311			A 3					21.82	
	MOTA	1312			A 3					22.81	
	MOTA	1313			A 3					22.95	
	ATOM	1314	CB	ALA	A 3	35 1 5.35	5 14.070	51.564	1.00	22.44	C

-153-

	ATOM	1315	N	ILE A 336	15.111	17.041	52.517	1.00 21.90	N
	MOTA	1316	CA	ILE A 336	14.827	18.022	53.560	1.00 22.98	С
	MOTA	1317	С	ILE A 336	13.822	19.050	53.038	1.00 23.92	С
_	MOTA	1318	0	ILE A 336	12.949	19.496	53.772	1.00 23.55	0
5	ATOM	1319	CB	ILE A 336	16.129	18.730	54.020	1.00 23.77	C
	MOTA	1320	CG1		17.021	17.724	54.753	1.00 24.24	C
	MOTA	1321	CG2		15.803	19.914	54.936	1.00 25.02	C
	MOTA	1322		ILE A 336	18.445	18.188	54.950	1.00 27.51	C
4.0	ATOM	1323	N	CYS A 337	13.942	19.411	51.765	1.00 22.82	N
10	MOTA	1324	CA	CYS A 337	13.020	20.365	51.166	1.00 23.92	C
	MOTA	1325	С	CYS A 337	11.582	19.846	51.235	1.00 24.00	C
	MOTA	1326	0	CYS A 337	10.665	20.577	51.605	1.00 25.45	0
	MOTA	1327	СВ	CYS A 337	13.410	20.622	49.705	1.00 22.95	C
4.5	MOTA	1328	SG	CYS A 337	12.289	21.736	48.817	1.00 25.85	S
15	MOTA	1329	N	ILE A 338	11.393	18.578	50.886	1.00 23.65	N
	MOTA	1330	CA	ILE A 338	10.070	17.957	50.890	1.00 23.56	C
	MOTA	1331	С	ILE A 338	9.457	17.814	52.284	1.00 26.02	C
	ATOM	1332	0	ILE A 338	8.288	18.153	52.501	1.00 25.70	0
00	MOTA	1333	CB	ILE A 338	10.126	16.560	50.231	1.00 23.28	C
20	ATOM	1334	CG1	ILE A 338	10.483	16.704	48.746	1.00 22.98	C
	MOTA	1335	CG2	ILE A 338	8.794	15.839	50.396	1.00 24.00	C
	MOTA	1336	CD1		10.807	15.387	48.057	1.00 22.98	C
	ATOM	1337	N	VAL A 339	10.242	17.305	53.225	1.00 26.29	N
25	ATOM	1338	CA	VAL A 339	9.754	17.106	54.584	1.00 29.21	C
25	ATOM	1339	C	VAL A 339	9.971	18.359	55.430	1.00 29.45	C
	ATOM	1340	0	VAL A 339	10.807	18.378	56.333	1.00 30.57	0
	ATOM	1341	CB	VAL A 339	10.461	15.901	55.241	1.00 30.37	C
	ATOM	1342		VAL A 339	9.751	15.516	56.524	1.00 31.20	C
30	MOTA	1343		VAL A 339	10.479	14.725	54.277	1.00 31.68	C
30	ATOM	1344	N	SER A 340	9.213	19.407	55.122	1.00 30.04	N
	MOTA	1345	CA	SER A 340	9.309	20.676	55.842	1.00 30.94	C
	ATOM	1346	C	SER A 340	8.061	20.868	56.701	1.00 31.69	C
	ATOM ATOM	1347 1348	O CB	SER A 340	6.940	20.841	56.195	1.00 31.64	
35	ATOM	1349	OG	SER A 340 SER A 340	9.438 10.664	21.838 21.773	54.853	1.00 32.39	
00	MOTA	1350	N	PRO A 341	8.243	21.773	54.142 58.013	1.00 35.78 1.00 32.38	0
	ATOM	1351	CA	PRO A 341	7.107	21.073	58.919	1.00 32.38	
	ATOM	1352	C	PRO A 341	6.344	22.579	58.774	1.00 35.82	
	ATOM	1353	Ö	PRO A 341	5.204	22.688	59.232	1.00 36.23	
40	ATOM	1354	СВ	PRO A 341	7.745	21.111	60.298	1.00 33.68	
••	ATOM	1355	CG	PRO A 341	9.110	21.675	60.094	1.00 33.78	
	ATOM	1356	CD	PRO A 341	9.517		58.754		
	ATOM	1357	N	ASP A 342	6.954	23.570	58.131	1.00 36.36	_
	MOTA	1358	CA	ASP A 342	6.301	24.866	57.981	1.00 37.82	
45	ATOM	1359	C	ASP A 342	5.580	25.094	56.657	1.00 38.30	
	ATOM	1360	Ō	ASP A 342	5.655	26.181	56.084	1.00 39.93	
	ATOM	1361	СВ	ASP A 342	7.304	26.001	58.213	1.00 39.62	
	ATOM	1362	CG	ASP A 342	8.441	25.987	57.218	1.00 41.16	
	ATOM	1363		ASP A 342	9.185	26.989	57.152	1.00 43.27	
50	ATOM	1364	OD2	ASP A 342	8.597	24.974	56.505	1.00 42.71	
	MOTA	1365	N	ARG A 343	4.887	24.072	56.170	1.00 37.31	
	MOTA	1366	CA	ARG A 343	4.123	24.195	54.933	1.00 37.10	
	MOTA	1367	C	ARG A 343	2.683	24.409	55.375	1.00 37.98	
	ATOM	1368	0	ARG A 343	2.198	23.723	56.273	1.00 38.15	
55	MOTA	1369	СВ	ARG A 343		22.911	54.103	1.00 35.71	
	MOTA	1370	CG	ARG A 343	5.595	22.543	53.612	1.00 32.83	
	ATOM	1371	CD	ARG A 343	6.123		52.565	1.00 31.70	
	MOTA	1372	NE	ARG A 343	7.282	22.947	51.879	1.00 29.77	N

-154-

								r1 000		0.05	^
	MOTA			ARG A		8.062	23.612		1.00 2		C
	MOTA			ARG A		7.818	24.886		1.00 2		N
	MOTA			ARG A		9.097	23.002		1.00 2		N
_	MOTA	1376		PRO A		1.979	25.367		1.00 3		N
5	ATOM	1377		PRO A		0.592	25.579	55.180	1.00 3		C
	ATOM	1378		PRO A		-0.279	24.351	54.924	1.00 3		C
	MOTA	1379	_	PRO A		-0.205	23.742	53.858	1.00 3		0
	MOTA	1380		PRO A		0.167	26.786	54.348	1.00 3		C
4.0	MOTA	1381		PRO A		0.974	26.624	53.092	1.00 4		C
10	MOTA	1382		PRO A		2.332	26.243	53.630	1.00 3		С
	ATOM	1383		GLY A		-1.085	23.978	55.912	1.00 3		N
	MOTA	1384		GLY A		-1.965	22.836	55.746	1.00 3		C
	MOTA	1385	-	GLY A		-1.567	21.544	56.437	1.00 3		C
	MOTA	1386		GLY A		-2.386	20.630	56.537	1.00		0
15	MOTA	1387	N	VAL A		-0.328	21.452	56.914	1.00		N
	MOTA	1388	CA	VAL A	346	0.125	20.234	57.585	1.00		С
	MOTA	1389	С	VAL A	346	-0.584	20.046	58.922	1.00		С
	MOTA	1390	0	VAL A		-0.832	21.012	59.643	1.00		0
	MOTA	1391	CB	VAL A	346	1.654	20.249	57.827	1.00		C
20	ATOM	1392	CG1	VAL A	346	2.383	20.409	56.503	1.00		C
	MOTA	1393	CG2	VAL A	346	2.030	21.366	58.784	1.00		C
	MOTA	1394	N	GLN A	347	-0.905	18.796	59.247	1.00		N
	MOTA	1395	CA	GLN A	347	-1.597	18.481	60.492	1.00		С
	ATOM	1396	C	GLN A	347	-0.631	18.135	61.612	1.00		С
25	MOTA	1397	0	GLN A	347	-0.657	18.758	62.673		39.58	0
	ATOM	1398	CB	GLN A	347	-2.564	17.314	60.280		43.00	C
	MOTA	1399	CG	GLN A	347	-3.565	17.531	59.157		47.50	C
	MOTA	1400	CD	GLN A	347	-4.526	18.678	59.423		50.27	C
	MOTA	1401	OE1	GLN A	347	-4.582	19.209	60.535		52.52	0
30	MOTA	1402	NE2	GLN A	347	-5.283	19.071	58.402		51.48	N
	ATOM	1403	N	ASP A	348	0.223	17.144	61.380		36.34	N
	MOTA	1404	CA	ASP A	348	1.181	16.730	62.398		35.34	C
	MOTA	1405	C	ASP A	348	2.568	17.313	62.152		33.83	C
	MOTA	1406	0	ASP A	348	3.474	16.622	61.679		33.85	0
35	ATOM	1407	CB	ASP A	348	1.257	15.203	62.458		34.84	C
	ATOM	1408	CG	ASP A	348	1.947	14.707	63.712		35.23	C
	ATOM	1409	OD1	ASP A	348	1.907	13.488	63.972		34.74	0
	ATOM	1410	OD2			2.531	15.539	64.437		34.97	0
	MOTA	1411	N	ALA A	349	2.727	18.587	62.492		32.41	N
40	MOTA	1412	CA	ALA A	349	3.991	19.286	62.307		32.51	С
	ATOM	1413	C	ALA A	349	5.122		63.121		32.68	С
	MOTA	1414	0	ALA A		6.263		62.662		32.47	0
	ATOM	1415	CB	ALA A		3.829		62.677		32.86	C
	ATOM	1416	N	ALA A	350	4.804				31.95	N
45	ATOM	1417	CA	ALA A	350	5.809				31.15	C
	MOTA	1418	С	ALA A	A 350	6.458				30.76	
	MOTA	1419	0	ALA A	A 350	7.676				30.22	
	MOTA	1420	СВ	ALA A	A 350	5.180				32.37	
	MOTA	1421	N	LEU A	A 351	5.643	15.510			30.64	
50	MOTA	1422	CA	LEU A	A 351	6.150				30.92	
	MOTA	1423		LEU A	A 351	7.032				30.72	
	ATOM	1424			A 351					30.35	
	ATOM	1425			A 351	4.989				32.92	
	ATOM	1426	CG	LEU 2	A 351	5.214				34.73	
55	ATOM	1427		1 LEU		4.073				35.25	
	MOTA	1428		2 LEU			3 11.640	62.005	1.00	36.86	C
	MOTA	1429			A 352		l 15.597	61.325	1.00	30.54	N
	ATOM	1430			A 352			60.158	1.00	29.35	C

-155-

	MOTA	1431	C	ILE A	352	8.628	16.646	60.580	1.00 2	9.73	C
	MOTA	1432	0	ILE A		9.658	16.371	59.959	1.00 3		0
	ATOM	1433	CB	ILE A	352	6.465	17.107	59.362	1.00 2	9.44	C
_	MOTA	1434	CG1	ILE A	352	5.175	16.463	58.842	1.00 2	9.58	C
5	MOTA	1435	CG2	ILE A	352	7.290	17.647	58.193	1.00 2	28.41	C
	MOTA	1436	CD1	ILE A	352	4.166	17.452	58.284	1.00 2	29.04	C
	ATOM	1437	N	GLU A		8.626	17.445	61.644	1.00 3	30.02	N
	ATOM	1438	CA	GLU A	353	9.857	18.058	62.130	1.00 3	30.56	C
	MOTA	1439	C	GLU 2	A 353	10.845	17.000	62.613	1.00 2	29.99	C
10	MOTA	1440	0	GLU A	A 353	12.050	17.147	62.438	1.00 2	29.97	0
	ATOM	1441	CB	GLU A	A 353	9.565	19.048	63.266	1.00 3	32.59	C
	MOTA	1442	CG	GLU Z	A 353	10.755	19.941	63.615	1.00 3	35.81	С
	MOTA	1443	CD	GLU A	A 353	10.462	20.922	64.740	1.00 3	38.69	С
	MOTA	1444	OE1		A 353	9.381	21.551	64.723	1.00 4	40.67	0
15	ATOM	1445	OE2		A 353	11.321	21.075	65.637	1.00 4		0
	ATOM	1446	N		A 354	10.334	15.935	63.223	1.00 2		N
	ATOM	1447	CA		A 354	11.191	14.861	63.716	1.00 2		C
	ATOM	1448	C		A 354	11.871	14.191	62.531	1.00 2		Č
	ATOM	1449	Ö		A 354	13.064	13.904	62.570	1.00		ŏ
20	ATOM	1450	СВ		A 354	10.367	13.843	64.491	1.00		Ċ
	ATOM	1451	N		A 355	11.100	13.940	61.478	1.00		N
	ATOM	1452	CA		A 355	11.638	13.314	60.274	1.00		c
	ATOM	1453	c		A 355	12.687	14.220	59.628	1.00		c
	ATOM	1454	ŏ		A 355	13.754	13.756	59.234	1.00		ŏ
25	ATOM	1455	СВ		A 355	10.514	13.730	59.259	1.00		č
	ATOM	1456	CG1		A 355	9.516	12.036	59.872	1.00		c
	ATOM	1457	CG2		A 355	11.101	12.458	57.964	1.00		C
	ATOM	1458	CD1		A 355	8.251	11.849	59.054	1.00		C
	ATOM	1459	N		A 356	12.398	15.515	59.534	1.00		N
30	ATOM	1460	CA		A 356		16.444	58.925		28.48	C
00	ATOM	1461	C		A 356		16.566	59.754		29.24	c
	ATOM	1462	Ö		A 356		16.622	59.202		27.50	ō
	ATOM	1463	СВ		A 356		17.833	58.739		28.93	c
	MOTA	1464	CG		A 356		18.753	57.823		29.68	C
35	ATOM	1465	CD		A 356		20.198	57.844		31.36	C
33			OE1								
	ATOM	1466			A 356		20.823	58.903		31.51	0
	MOTA	1467 1468	NE2		A 356		20.742 16.613	56.667		29.52	N
	MOTA		N		A 357			61.078 61.945			N
40	ATOM	1469	CA		A 357		16.724 15.550			30.44	C
40	ATOM	1470	C		A 357			61.739		29.70	C
	ATOM	1471	0		A 357		15.729	61.727		30.37	0
	ATOM	1472	CB		A 357		16.791	63.423		32.83	C
	ATOM	1473	CG		A 357		18.141	63.812		34.76	C
AE	MOTA	1474			A 357		19.110	63.040		36.63	0
45	ATOM	1475			A 357		18.236	64.905		36.89	0
	MOTA	1476	N		A 358		14.351	61.577		30.08	N
	ATOM	1477	CA		A 358		13.167	61.368		30.11	C
	MOTA	1478	C		A 358		13.309	60.073		29.92	C
50	MOTA	1479	0		A 358		12.880	59.996		29.08	0
50	MOTA	1480	СВ		A 358		11.906	61.323		31.17	С
	MOTA	1481	CG		A 358		10.608	61.149		33.90	С
	MOTA	1482	CD		A 358		9.382	61.402		36.03	С
	MOTA	1483	NE		A 358		9.299	60.479		38.00	N
	ATOM	1484	CZ		A 358		8.358	60.533		39.39	С
55	ATOM	1485	NH1		A 358		7.417	61.469		39.22	N
	MOTA	1486	NH2	2 ARG	A 358	12.858	8.353	59.653	1.00	39.21	N
	MOTA	1487	N	LEU	A 359		13.919	59.061	1.00	28.41	N
	MOTA	1488	CA		A 359					27.76	С

-156-

	N/ON	1489	~	LEU A	2	E 0	18.757	15.255	57.890	1.00 2	7 90	С
	ATOM			LEU A			19.853	15.233	57.338	1.00 2		Ö
	ATOM	1490										
	MOTA	1491		LEU A			16.704	14.482	56.697	1.00		C
_	MOTA	1492		LEU A			15.646	13.421	56.384	1.00		C
5	MOTA	1493		LEU A			14.593	13.994	55.448	1.00		C
	MOTA	1494	CD2	LEU A			16.310	12.210	55.758	1.00		C
	MOTA	1495	N	SER A	3	60	18.393	16.312	58.610	1.00		N
	MOTA	1496	CA	SER A	١ 3	60	19.288	17.448	58.790	1.00	30.04	C
	ATOM	1497	C	SER A	A 3	60	20.540	17.046	59.561	1.00	30.70	C
10	MOTA	1498	0	SER A	A 3	60	21.647	17.454	59.212	1.00	31.03	0
	ATOM	1499	СВ	SER A			18.573	18.578	59.534	1.00	32.12	C
	ATOM	1500	OG	SER A	A 3	60	17.496	19.084	58.765	1.00	36.13	0
	ATOM	1501	N	ASN A			20.367	16.251	60.613	1.00		N
	ATOM	1502	CA	ASN A			21.513	15.816	61.405	1.00		C
15	MOTA	1502	C	ASN A			22.417	14.921	60.570	1.00		Č
13								14.935	60.728		31.06	Ö
	MOTA	1504	0	ASN A			23.637				34.28	
	MOTA	1505	CB	ASN A			21.055	15.083	62.667			C
	MOTA	1506	CG	ASN A			20.328	15.998	63.637		37.26	C
	MOTA	1507		ASN 2			20.736	17.139	63.854		39.61	0
20	MOTA	1508	ND2				19.252	15.497	64.234		39.64	N
	MOTA	1509	N	THR .			21.815	14.146	59.674		29.26	N
	MOTA	1510	CA	THR .	A :	362	22.583	13.270	58.800	1.00	28.14	C
	MOTA	1511	С	THR .	A :	362	23.419	14.135	57.863	1.00	27.56	C
	ATOM	1512	0	THR .	A :	362	24.607	13.879	57.654	1.00	27.15	0
25	ATOM	1513	CB	THR	A :	362	21.654	12.371	57.956	1.00	28.47	C
	ATOM	1514	OG1	THR	A :	362	20.923	11.495	58.823	1.00	28.00	0
	ATOM	1515	CG2				22.461	11.548	56.955	1.00	27.60	C
	MOTA	1516	N	LEU			22.795	15.167	57.301	1.00	26.97	N
	ATOM	1517	CA	LEU			23.493	16.064	56.388		27.40	C
30	ATOM	1518	C	LEU			24.623	16.798	57.100		28.23	Č
00		1519	Ö	LEU			25.736	16.884	56.588		27.96	ŏ
	ATOM		СВ				22.519	17.089	55.782		26.59	c
	ATOM	1520	_	LEU							26.54	c
	ATOM	1521	CG	LEU			23.153	18.156	54.882			
25	MOTA	1522		LEU			23.829	17.495	53.687		26.43	C
35	MOTA	1523	CD2				22.090	19.142	54.417		26.28	С
	MOTA	1524	N	GLN			24.340	17.325	58.286		29.48	N
	MOTA	1525	CA	GLN			25.360	18.054	59.029		31.77	С
	MOTA	1526	C	GLN			26.530	17.140	59.399		30.91	C
	MOTA	1527	0	GLN	Α	364	27.691	17.539	59.307		30.91	0
40	ATOM	1528	CB	GLN	Α	364	24.747	18.681	60.283		33.97	C
	ATOM	1529	CG	GLN	A	364	25.579	19.812	60.870	1.00	39.97	C
	ATOM	1530	CD	GLN	A	364	24.749	20.793	61.681	1.00	41.73	С
	ATOM	1531	OE1	GLN	Α	364	25.270	21.785	62.190	1.00	45.56	0
	MOTA	1532		GLN			23.452	20.523	61.800	1.00	43.48	N
45	ATOM	1533	N	THR			26.224	15.910	59.799	1.00	30.38	N
	ATOM	1534	CA	THR			27.263	14.956	60.176	1.00	30.54	С
	ATOM	1535	C	THR			28.099	14.561	58.965		29.67	C
	ATOM	1536	ŏ	THR			29.319	14.454	59.054		30.84	ō
	ATOM	1537	СВ	THR			26.658	13.687	60.802		30.66	Č
50							25.883	14.045			32.31	ŏ
50	ATOM	1538	OG1								31.16	
	ATOM	1539	CG				27.759	12.728				C
	MOTA	1540				366	27.437	14.348			29.11	N
	MOTA	1541				366	28.131	13.976			28.71	C
	MOTA	1542				366		15.051			28.75	С
55	MOTA	1543				366					29.49	0
	MOTA	1544	CB	TYR	Α	366	27.122			1.00	27.69	С
	MOTA	1545	CG	TYR	A	366	27.779	13.396	54.148	1.00	27.26	С
	MOTA	1546		1 TYR				14.421	53.313	1.00	27.40	С

-157-

	ATOM	1547	CD2	TYR A	366	28.017	12.079	53.759	1.00 2	7.61	C
	MOTA	1548	CE1	TYR A	366	28.912	14.144	52.130	1.00 2	8.23	C
	ATOM	1549	CE2	TYR A	366	28.697	11.790	52.578	1.00 2	8.00	C
	MOTA	1550	CZ	TYR A	366	29.143	12.825	51.770	1.00 2	8.28	C
5	MOTA	1551	OH	TYR A	366	29.838	12.546	50.615	1.00 2	8.34	0
	MOTA	1552	N	ILE A	367	28.692	16.310	56.174	1.00 3	0.76	N
	ATOM	1553	CA	ILE A	367	29.559	17.412	55.762	1.00 3		C
	MOTA	1554	С	ILE A	367	30.823	17.533	56.614	1.00 3	5.15	C
	MOTA	1555	0	ILE A	367	31.924	17.688	56.086	1.00 3		0
10	MOTA	1556	CB	ILE A	367	28.805	18.763	55.807	1.00 3	2.16	С
	MOTA	1557	CG1	ILE A	367	27.685	18.764	54.763	1.00 3		C
	MOTA	1558	CG2	ILE A	367	29.769	19.915	55.535	1.00 3		C
	MOTA	1559	CD1	ILE A	367	26.790	19.977	54.829	1.00 3		C
	MOTA	1560	N	ARG A	368	30.660	17.465	57.930	1.00 3		N
15	MOTA	1561	CA	ARG A	368	31.794	17.582	58.842	1.00 4	1.56	C
	MOTA	1562	C	ARG A	368	32.749	16.406	58.711	1.00 4		С
	ATOM	1563	0	ARG A		33.963	16.558	58.845	1.00 4		0
	ATOM	1564	CB	ARG A		31.309	17.652	60.289	1.00 4		С
	MOTA	1565	CG	ARG A	368	30.469	18.868	60.627	1.00 4		C
20	MOTA	1566	CD	ARG A	368	30.023	18.814	62.081	1.00 5		C
	MOTA	1567	NE	ARG A	368	29.222	17.621	62.348	1.00 5		N
	MOTA	1568	CZ	ARG A		28.703	17.315	63.531	1.00 5		С
	MOTA	1569	NH1	ARG A		28.901	18.117	64.570	1.00 5		N
	ATOM	1570	NH2	ARG A		27.983	16.210	63.676	1.00 5		N
25	ATOM	1571	N	CYS A		32.187	15.234	58.440	1.00 4		N
	MOTA	1572	CA	CYS A		32.964	14.011	58.333	1.00 4		C
	MOTA	1573	С	CYS A		33.501	13.644	56.949	1.00 4		С
	MOTA	1574	0	CYS A		34.641	13.198	56.828	1.00		0
00	MOTA	1575	CB		A 369	32.128	12.848	58.881	1.00		С
30	MOTA	1576	SG		A 369	32.925	11.238	58.816	1.00 !		S
	MOTA	1577	N		A 370	32.700	13.841	55.905	1.00		N
	MOTA	1578	CA		A 370	33.123	13.457	54.558	1.00		C
	MOTA	1579	C		A 370	33.451	14.563	53.559	1.00		C
25	MOTA	1580	0		A 370	34.058	14.292	52.520	1.00		0
35	MOTA	1581	CB		A 370	32.068	12.533	53.940	1.00		C
	ATOM	1582	CG		A 370	31.827	11.248	54.719	1.00		C
	MOTA	1583	CD		A 370	33.034	10.323	54.660	1.00		C
	MOTA	1584	NE		A 370	32.881	9.160	55.532	1.00 1.00		N
40	MOTA	1585	CZ		A 370	31.913	8.254	55.420 54.465		54.23	N
40	MOTA	1586		ARG		30.999 31.857	8.367 7.236	56.268		54.23	N
	MOTA	1587 1588		ARG	A 370 A 371		15.799	53.845	1.00		N
	MOTA		N				16.879	52.908		47.01	C
	MOTA	1589	CA		A 371 A 371		17.554	53.217		47.99	Č
45	MOTA	1590	C		A 371		18.227	54.237		46.99	Ö
40	ATOM	1591 1592	O CB		A 371					45.11	Č
	ATOM	1593	CG		A 371			51.659		44.21	č
	MOTA	1594		HIS						43.28	N
	MOTA	1595		HIS						43.81	C
50	ATOM ATOM	1596		HIS						43.79	C
30	ATOM	1597		HIS						43.86	
	ATOM	1598			A 372					49.67	
	ATOM	1599			A 372					51.25	
	ATOM	1600			A 372					52.68	
55	MOTA	1601			A 372					52.39	
	ATOM	1602			A 372					51.31	
	MOTA	1602			A 372					51.05	
	ATOM	1604			A 372					50.21	
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-158-

	MOTA	1605	N	PRO A	. 3	73	37.961	20.187	52.914	1.00	54.03	N
	MOTA	1606	CA	PRO A	٠ 3	73	38.107	21.640	52.777		55.28	C
	MOTA	1607	-	PRO A			38.693	22.028	51.420		56.14	С
_	MOTA	1608		PRO A			39.284	21.197	50.731		56.44	0
5	MOTA	1609		PRO A			39.036	21.998	53.932		55.37	C
	MOTA	1610	CG	PRO P			39.925	20.793	54.011		55.24	C
	MOTA	1611	CD	PRO A			38.934	19.653	53.885		54.59	C
	MOTA	1612	N	PRO A			38.535	23.299	51.017		56.81	N
	ATOM	1613	CA	PRO A			37.848	24.368	51.750		57.49	C
10	ATOM	1614	C	PRO A			36.324	24.301	51.617		57.83	C
	ATOM	1615	0	PRO A			35.642	24.299	52.664		58.58	0
	MOTA	1616	CB	PRO A			38.431	25.631	51.127		57.24	C
	ATOM	1617	CG	PRO A			38.601	25.226	49.698		57.37	C
	MOTA	1618	CD	PRO A			39.194	23.834	49.811		57.05	С
15	ATOM	1619	N	LEU !			30.279	26.156	57.018		49.88	N
	ATOM	1620	CA	LEU A			29.679	27.221	56.220		45.66	C
	MOTA	1621	С	LEU A			28.825	26.586	55.127		41.60	С
	MOTA	1622	0	LEU A			27.802	27.138	54.723		38.14	0
	MOTA	1623	CB	LEU A			30.769	28.092	55.590		53.84	C
20	ATOM	1624	CG	LEU A			30.382	29.273	54.702		57.56	C
	MOTA	1625		LEU A			29.709	30.349	55.545		59.64	C
	MOTA	1626		LEU 2			31.634	29.822	54.017		59.59	С
	MOTA	1627	N	LEU .			29.370	25.200	54.660		35.28	N
	MOTA	1628	CA	LEU :			28.529	24.615	53.626		33.21	C
25	MOTA	1629	С	LEU .			27.095	24.355	54.080		32.24	С
	MOTA	1630	0	LEU .			26.157	24.594	53.325		31.09	0
	MOTA	1631	CB	LEU			29.151	23.309	53.121		33.21	C
	MOTA	1632	CG	LEU			28.379	22.603	52.003		31.83	С
	MOTA	1633		LEU			28.301	23.508	50.783		33.04	C
30	MOTA	1634	CD2				29.066	21.292	51.651		32.12	С
	MOTA	1635	N	TYR			26.917	23.869	55.304		31.72	N
	MOTA	1636	CA	TYR			25.572	23.588	55.792		32.34	С
	MOTA	1637	C	TYR			24.717	24.852	55.780		32.63	C
0.5	MOTA	1638	0	TYR			23.562	24.833	55.339		31.56	0
35	MOTA	1639	CB	TYR			25.611	23.008	57.208		33.03	C
	MOTA	1640	CG	TYR			24.239	22.659	57.743		34.66	C
	ATOM	1641	CD1				23.486	21.635	57.169	1.00		C
	ATOM	1642	CD2				23.680	23.373	58.800	1.00		C
40	MOTA	1643	CE1				22.209	21.333	57.636		36.98	C
40	MOTA	1644	CE2				22.410	23.080	59.274		36.43	C
	MOTA	1645	CZ	TYR			21.679	22.060	58.688		37.93	C
	ATOM	1646	ОН	TYR			20.420		59.154		38.77	0
	MOTA	1647	N	ALA			25.288	25.950	56.266		32.03	N
45	ATOM	1648	CA	ALA				27.223	56.304		32.04 31.59	С
45	ATOM	1649	C	ALA			24.190	27.683	54.902			C
	ATOM	1650	0	ALA				28.187	54.693		32.20 32.84	0
	ATOM	1651	СВ	ALA				28.287	56.981		30.09	C N
	ATOM	1652	N	LYS				27.515 27.916	53.948 52.570		30.96	
50	MOTA	1653	CA	LYS							30.98	
50	MOTA	1654	C	LYS				27.083	51.943			
	MOTA	1655	0	LYS				27.575 27.781	51.101		30.60 31.98	
	MOTA	1656	CB	LYS				28.757	51.731		31.96 34.76	
	ATOM	1657	CG	LYS								
E.E.	MOTA	1658	CD	LYS) 38.05) 39.31	
55	MOTA	1659	CE	LYS							39.31 41.47	
	ATOM	1660		LYS								
	ATOM	1661		MET							29.65	
	MOTA	1662	CA	MET	Α	383	22.621	24.923	51.821	T.00	29.41	. C

-159-

	MOTA	1663	-	MET A		21.253	25.286		1.00 29.82	C
	MOTA	1664		MET A		20.250	25.271	51.677	1.00 29.12	0
	MOTA	1665		MET A	-	22.958	23.468	52.165	1.00 28.17	C
_	MOTA	1666		MET A		24.130	22.908	51.381	1.00 28.12	C
5	MOTA	1667		MET A		24.510	21.186	51.776	1.00 28.48	S
	ATOM	1668	CE	MET A	383	23.099	20.338	51.048	1.00 28.89	C
	ATOM	1669		ILE A		21.215	25.612	53.676	1.00 30.76	N
	MOTA	1670	CA	ILE A	384	19.960	25.983	54.319	1.00 32.84	С
	MOTA	1671	C	ILE A	384	19.422	27.271	53.701	1.00 32.96	C
10	MOTA	1672	0	ILE A		18.208	27.458	53.594	1.00 32.83	0
	MOTA	1673	CB	ILE A		20.149	26.186	55.842	1.00 34.53	C
	ATOM	1674	CG1	ILE A	384	20.651	24.889	56.482	1.00 36.66	C
	ATOM	1675		ILE A		18.834	26.610	56.482	1.00 36.24	C
	ATOM	1676	CD1	ILE A	384	19.744	23.691	56.257	1.00 37.66	C
15	ATOM	1677	N	GLN A	385	20.328	28.153	53.287	1.00 32.82	N
	MOTA	1678	CA	GLN A	385	19.931	29.412	52.669	1.00 33.03	С
	MOTA	1679	С	GLN A	385	19.288	29.174	51.303	1.00 32.26	С
	ATOM	1680	0	GLN A	385	18.382	29.905	50.901	1.00 30.38	
	ATOM	1681	СВ	GLN A	385	21.136	30.342	52.515	1.00 35.19	
20	MOTA	1682	CG	GLN A	385	20.839	31.588	51.692	1.00 39.54	
	ATOM	1683	CD	GLN A	385	19.705	32.421	52.270	1.00 41.95	
	ATOM	1684	OE1	GLN A	385	19.024	33.151	51.545	1.00 44.07	0
	ATOM	1685	NE2	GLN A	385	19.504	32.324	53.579	1.00 42.90	
	MOTA	1686	N	LYS A	A 386	19.756	28.152	50.591	1.00 30.96	
25	MOTA	1687	CA	LYS 2	A 386	19.197	27.840	49.282	1.00 30.88	
	ATOM	1688	С	LYS A	A 386	17.748	27.415	49.447	1.00 29.98	
	ATOM	1689	0	LYS 2	A 386	16.927	27.635	48.558	1.00 29.72	
	MOTA	1690	CB	LYS 2	A 386	19.985	26.719	48.601	1.00 32.29	
	ATOM	1691	CG	LYS 2	A 386	21.430	27.064	48.310	1.00 35.09	
30	ATOM	1692	CD	LYS :	A 386	21.539	28.305	47.453	1.00 36.92	
	MOTA	1693	CE	LYS .	A 386	22.997	28.643	47.170	1.00 39.17	7 C
	MOTA	1694	NZ	LYS	A 386	23.133	30.008	46.589	1.00 40.63	
	MOTA	1695	N	LEU	A 387	17.433	26.804	50.583	1.00 29.25	
	ATOM	1696	CA	LEU	A 387	16.064	26.373	50.833	1.00 29.50	
35	ATOM	1697	С	LEU	A 387	15.172	27.604	50.982	1.00 29.30	
	MOTA	1698	0	LEU	A 387	14.014	27.594	50.572	1.00 27.98	
	ATOM	1699	CB	LEU	A 387	15.988	25.503	52.091	1.00 30.49	
	MOTA	1700	CG	LEU	A 387	16.625		51.980	1.00 31.0	
	ATOM	1701	CD1	. LEU	A 387	16.443	23.363	53.289	1.00 33.0	
40	MOTA	1702	CD2	LEU	A 387	15.985	23.339	50.839	1.00 31.2	7 C
	MOTA	1703	N	ALA	A 388	15.714	28.667	51.566	1.00 28.7	
	ATOM	1704	CA	ALA	A 388	14.952	29.903	51.735	1.00 29.5	
	ATOM	1705	С		A 388		30.557	50.367	1.00 29.6	
	ATOM	1706	0	ALA	A 388	13.696	31.121	50.082	1.00 29.6	
45	ATOM	1707	CB	ALA	A 388	15.687	30.856	52.679	1.00 30.0	
	MOTA	1708	N	ASP	A 389	15.786	30.479	49.524	1.00 29.6	
	MOTA	1709	CA	ASP	A 389	15.730	31.044	48.175	1.00 30.0	
	ATOM	1710		ASP	A 389	14.625	30.360	47.378		
	MOTA	1711		ASP	A 389	13.917	31.000	46.598		
50	ATOM	1712	CB	ASP	A 389	17.059				
	MOTA	1713		ASP	A 389	18.183	31.682			
	ATOM	1714			A 389					
	ATOM	1715			A 389		32.608	48.796		
	ATOM	1716			A 390		29.052	47.572		
55	ATOM	1717			A 390					
	MOTA	1718			A 390		7 28.730	47.223		
	ATOM	1719			A 390			46.360	1.00 26.9	
	MOTA	1720			A 390			47.252	1.00 28.8	37 C

-160-

	MOTA	1721	CG	LEU A	390	14.130	25.761	46.221	1.00		C
	MOTA	1722	CD1	LEU A	390	14.754	26.424	45.017	1.00	31.00	C
	MOTA	1723	CD2	LEU A	390	15.101	24.810	46.902	1.00	31.75	C
	MOTA	1724	N	ARG A	391	11.849	29.109	48.481	1.00	27.87	N
5	ATOM	1725	CA	ARG A	391	10.535	29.574	48.917	1.00	28.52	C
	ATOM	1726	С	ARG A		10.132	30.808	48.125	1.00	28.78	C
	MOTA	1727	0	ARG A		8.968	30.961	47.757	1.00		0
	MOTA	1728	СВ	ARG A		10.536	29.919	50.415	1.00		C
	MOTA	1729	CG	ARG A		10.795	28.744	51.354		32.51	Ċ
10	ATOM	1730	CD	ARG A		9.743	27.658	51.208	1.00		c
••	ATOM	1731	NE	ARG A		9.952	26.552	52.141	1.00		N
	MOTA	1732	CZ	ARG A		9.395	26.460	53.346	1.00		Č
				ARG A		8.580	27.411	53.783	1.00		N
	ATOM	1733									
15	MOTA	1734	NH2	ARG A		9.646	25.408	54.115	1.00		N
15	ATOM	1735	N	SER A		11.094	31.690	47.865	1.00		N
	MOTA	1736	CA	SER A		10.811	32.908	47.114	1.00		C
	ATOM	1737	С	SER A		10.483	32.588	45.664		28.02	C
	MOTA	1738	0	SER A		9.577	33.178	45.082		28.38	0
	MOTA	1739	CB	SER A		11.997	33.866	47.185		31.21	С
20	MOTA	1740	OG	SER A	392	12.192	34.305	48.518		37.19	0
	MOTA	1741	N	LEU A	393	11.219	31.648	45.081	1.00	26.23	N
	MOTA	1742	CA	LEU A	393	10.972	31.253	43.700	1.00	26.10	C
	MOTA	1743	C	LEU A	393	9.614	30.567	43.586	1.00	25.57	C
	ATOM	1744	0	LEU A	393	8.919	30.705	42.576	1.00	26.87	0
25	ATOM	1745	CB	LEU A	393	12.081	30.309	43.216	1.00	26.02	C
	ATOM	1746	CG	LEU A		13.450	30.968	43.030	1.00	26.66	C
	ATOM	1747		LEU A	393	14.536	29.905	42.878	1.00	28.52	С
	ATOM	1748		LEU A		13.400	31.869	41.808		29.45	C
	ATOM	1749	N	ASN A		9.242	29.825	44.625		24.50	N
30	ATOM	1750	CA	ASN A		7.964	29.122	44.656		26.07	C
	ATOM	1751	C	ASN A		6.855	30.167	44.570		27.28	c
	ATOM	1752	ŏ	ASN A		5.929	30.055	43.764		26.29	ŏ
	ATOM	1753	СВ	ASN A		7.827	28.347	45.967		26.75	C
	ATOM	1754	CG	ASN A		6.646	27.397	45.968		28.26	Č
35	ATOM	1755	OD1			5.660	27.604	45.263		28.24	o
00						6.736	26.352	46.779		28.79	
	MOTA	1756	ND2				31.188				N
	MOTA	1757	N	GLU A		6.966		45.413		28.62 30.55	N
	MOTA	1758	CA	GLU A		5.986	32.266	45.464			C
40	MOTA	1759	C	GLU A		5.815	32.976	44.130		29.66	C
40	ATOM	1760	0	GLU A		4.691	33.213	43.684		29.50	0
	MOTA	1761	CB	GLU A		6.385	33.280	46.536		33.44	C
	MOTA	1762	CG	GLU A		6.277	32.744	47.954		40.01	C
	MOTA	1763	CD	GLU A		4.838	32.481	48.366		44.38	С
45	MOTA	1764		GLU A		4.618	32.045	49.518		46.89	0
45	MOTA	1765	OE2	GLU A		3.924	32.713	47.540		46.99	0
	MOTA	1766	N	GLU A		6.929	33.324	43.496		29.08	N
	MOTA	1767	CA	GLU A	396	6.871	34.013	42.217	1.00	28.78	C
	ATOM	1768	С	GLU A	396	6.280	33.102	41.148	1.00	28.20	C
	ATOM	1769	0	GLU A	396	5.486	33.545	40.317	1.00	27.96	0
50	MOTA	1770	CB	GLU A	396	8.265	34.490	41.791	1.00	30.45	С
	MOTA	1771	CG	GLU A	396	8.276	35.254	40.465	1.00	30.29	C
	ATOM	1772	CD	GLU A		7.502	36.568	40.525	1.00	33.32	С
	ATOM	1773		GLU F		7.098	37.068	39.452		32.46	0
	ATOM	1774	OE2			7.307	37.108	41.639		32.27	ō
55	ATOM	1775	N	HIS A		6.651	31.826	41.162		26.94	N
	ATOM	1776	CA	HIS A		6.104	30.919	40.162		27.05	
	ATOM	1777	C	HIS A		4.583	30.835	40.295		27.50	
										27.05	
	ATOM	1778	0	HIS A	3 29/	3.866	30.834	39.294	1.00	27.05	J

-161-

	ATOM	1779	СВ	HIS A 397	6.718	29.519	40.282	1.00 26.64	C
	MOTA	1780	CG	HIS A 397	6.058	28.507	39.400	1.00 26.04	1 C
	ATOM	1781	ND1	HIS A 397	4.999	27.731	39.822	1.00 27.22	2 N
	MOTA	1782	CD2	HIS A 397	6.227	28.228	38.086	1.00 26.30	5 C
5	ATOM	1783	CE1	HIS A 397	4.542	27.024	38.805	1.00 26.59	9 C
	ATOM	1784	NE2	HIS A 397	5.268	27.308	37.740	1.00 26.30	N C
	MOTA	1785	N	SER A 398	4.094	30.785	41.529	1.00 28.0	4 N
	MOTA	1786	CA	SER A 398	2.657	30.696	41.775	1.00 29.6	2 C
	ATOM	1787	C	SER A 398	1.921	31.901	41.195	1.00 29.8	7 C
10	ATOM	1788	0	SER A 398	0.862	31.761	40.579	1.00 28.3	2 0
	ATOM	1789	CB	SER A 398	2.389	30.604	43.279	1.00 31.4	4 C
	MOTA	1790	OG	SER A 398	1.000	30.483	43.534	1.00 38.7	2 0
	ATOM	1791	N	LYS A 399	2.485	33.085	41.397	1.00 30.0	6 N
	MOTA	1792	CA	LYS A 399	1.882	34.313	40.885	1.00 31.6	1 C
15	ATOM	1793	С	LYS A 399	1.807	34.283	39.363	1.00 30.9	1 C
	ATOM	1794	0	LYS A 399	0.790	34.651	38.771	1.00 30.2	1 0
	MOTA	1795	CB	LYS A 399	2.698	35.527	41.336	1.00 33.7	9 C
	ATOM	1796	CG	LYS A 399	2.754	35.693	42.842	1.00 38.6	3 C
	MOTA	1797	CD	LYS A 399	3.521	36.946	43.236	1.00 41.4	8 C
20	MOTA	1798	CE	LYS A 399	3.571	37.101	44.750	1.00 43.5	7 C
	MOTA	1799	NZ	LYS A 399	4.340	38.313	45.155	1.00 44.9	0 N
	MOTA	1800	N	GLN A 400	2.886	33.834	38.731	1.00 29.2	0 N
	ATOM	1801	CA	GLN A 400	2.926	33.770	37.278	1.00 28.7	8 C
	MOTA	1802	С	GLN A 400	2.052	32.660	36.702	1.00 27.9	5 C
25	ATOM	1803	0	GLN A 400	1.524	32.789	35.595	1.00 27.6	4 0
	MOTA	1804	CB	GLN A 400	4.374	33.637	36.802	1.00 28.4	9 C
	MOTA	1805	CG	GLN A 400	5.147	34.942	36.964	1.00 30.6	4 C
	MOTA	1806	CD	GLN A 400	6.483	34.940	36.256	1.00 31.3	4 C
	MOTA	1807	OE1	GLN A 400	6.673	34.235	35.265	1.00 33.9	0 0
30	ATOM	1808	NE2	GLN A 400	7.414	35.751	36.749	1.00 31.0	2 N
	ATOM	1809	N	TYR A 401	1.894	31.571	37.446	1.00 26.5	6 N
	ATOM	1810	CA	TYR A 401	1.051	30.481	36.980	1.00 27.3	11 C
	ATOM	1811	С	TYR A 401	-0.382	30.998	36.941	1.00 27.9	98 C
	ATOM	1812	0	TYR A 401	-1.147	30.686	36.024	1.00 27.2	25 O
35	ATOM	1813	CB	TYR A 401	1.127	29.285	37.931	1.00 27.7	
	ATOM	1814	CG	TYR A 401	0.229	28.147	37.516	1.00 27.4	
	MOTA	1815	CD1	TYR A 401	0.600	27.281	36.489	1.00 28.3	38 C
	ATOM	1816	CD2	TYR A 401	-1.013	27.960	38.119	1.00 29.2	
	ATOM	1817		TYR A 401	-0.242	26.260	36.068	1.00 28.4	
40	MOTA	1818	-	TYR A 401	-1.868	26.938	37.703	1.00 29.0	
	MOTA	1819	CZ	TYR A 401	-1.475	26.094	36.677	1.00 29.9	95 C
	MOTA	1820	OH	TYR A 401	-2.319		36.252	1.00 30.3	
	MOTA	1821	N	ARG A 402	-0.742	31.790	37.948	1.00 29.3	
	MOTA	1822	CA	ARG A 402	-2.083	32.360	38.021	1.00 32.	
45	MOTA	1823	С	ARG A 402	-2.386	33.173	36.769	1.00 32.	
	MOTA	1824	0	ARG A 402	-3.434	32.998	36.150	1.00 31.	
	MOTA	1825	СВ	ARG A 402		33.251	39.256	1.00 36.	
	MOTA	1826	CG	ARG A 402			39.391	1.00 41.	
	MOTA	1827	CD	ARG A 402			40.669	1.00 45.	
50	MOTA	1828	NE	ARG A 402			41.873	1.00 49.	
	ATOM	1829	CZ	ARG A 402			42.410	1.00 51.	
	MOTA	1830		L ARG A 402				1.00 52.	
	MOTA	1831		2 ARG A 402					
	ATOM	1832	N	CYS A 403				1.00 32.	
55	MOTA	1833		CYS A 403					
	MOTA	1834		CYS A 403					
	MOTA	1835		CYS A 403					
	ATOM	1836	СВ	CYS A 403	-0.450	35.838	35.030	1.00 35.	60 C

-162-

	MOTA	1837	SG	CYS A		-0.253	36.492	33.340	1.00 4		S
	MOTA	1838	N	LEU A		-0.950	32.980	33.911	1.00 3		N
	MOTA	1839	CA	LEU A		-0.967	32.065	32.784	1.00 3		C
_	MOTA	1840	С	LEU A		-2.327	31.390	32.638	1.00 2		C
5	MOTA	1841	0	LEU A		-2.840	31.256	31.529	1.00 3		0
	MOTA	1842	CB	LEU A		0.130	31.008	32.955	1.00 3		C
	MOTA	1843	CG	LEU A		0.353	30.078	31.766	1.00 3		C
	MOTA	1844		LEU A		0.840	30.895	30.580	1.00 3		C
	MOTA	1845	CD2	LEU A		1.370	29.005	32.127	1.00 3		C
10	MOTA	1846	N	SER A		-2.918	30.987	33.760	1.00 2		N
	MOTA	1847	CA	SER A		-4.212	30.309	33.749	1.00 2		C
	MOTA	1848	С	_	4 405		31.173	33.218	1.00 2		C
	MOTA	1849	0		4 405		30.651	32.885	1.00 2		0
	MOTA	1850	CB		4 405		29.802	35.153	1.00 3		C
15	MOTA	1851	OG		4 405		30.873	36.040	1.00 3		0
	MOTA	1852	N		4 406		32.484	33.145	1.00 2		N
	MOTA	1853	CA		A 406		33.396	32.636	1.00 2		C
	MOTA	1854	C		A 406		33.340	31.112	1.00 2		C
	MOTA	1855	0		A 406		33.778	30.518	1.00 2		0
20	MOTA	1856	CB		A 406		34.842	33.042	1.00 2		C
	MOTA	1857	CG		A 406		35.128	34.503	1.00 2		C
	ATOM	1858		PHE .			36.196	35.099	1.00 2		C
	MOTA	1859		PHE .			34.361	35.278	1.00 2		С
	MOTA	1860		PHE			36.494	36.446	1.00		С
25	MOTA	1861		PHE			34.651	36.632	1.00		C
	MOTA	1862	CZ		A 406		35.719	37.214	1.00		С
	MOTA	1863	N		A 407		32.814	30.478	1.00		N
	MOTA	1864	CA		A 407		32.748	29.019	1.00		С
20	MOTA	1865	C		A 407		31.687	28.500	1.00		C
30	ATOM	1866	0		A 407		30.524	28.903	1.00		0
	ATOM	1867	CB		A 407		32.448	28.527	1.00		C
	MOTA	1868	CG		A 407		32.694	27.030	1.00		C
	MOTA	1869	CD		A 407		34.165	26.651	1.00		C
25	ATOM	1870		GLN			34.494	25.520	1.00		0
35	MOTA	1871		GLN			35.052	27.590	1.00		N
	ATOM	1872	N		A 408		32.079	27.608	1.00		N
	MOTA	1873	CA		A 40		31.124	27.058	1.00		C
	MOTA	1874	C		A 40		29.913	26.398	1.00		C
40	MOTA	1875	0		A 40		30.056	25.688	1.00		0
40	MOTA	1876	CB		A 40	-	31.967	26.054		25.96	C
	ATOM	1877	CG		A 40		33.331 33.449	26.690		25.60	C
	MOTA	1878	CD		A 40					26.30 31.66	C
	ATOM	1879	N		A 40		28.731	26.646	_		N
45	MOTA	1880	CA		A 40			26.078		34.64 34.56	C
40	MOTA	1881	C		A 40			26.661 26.122		34.24	C 0
	MOTA	1882	0		A 40			24.555		37.88	
	MOTA	1883	CB		A 40					43.65	C
	MOTA	1884	CG		A 40 A 40			23.823 23.887		46.69	C
50	MOTA	1885	CD		A 40			24.998		49.95	0
30	MOTA	1886 1887	OE:			9 -10.252 9 -10.153		22.821		49.48	Ö
	ATOM				A 41			27.759		33.81	N
	ATOM	1888	N CA					28.382		35.08	C
	ATOM	18 8 9 1890	CA		A 41 A 41			29.002		34.78	C
55	MOTA MOTA	1890	0		A 41			28.943		34.78	
55	ATOM	1892	СВ		A 41			29.455		36.13	C
	ATOM	1893	SG		A 41			30.271		41.53	s
		1893			A 41			29.593		34.62	
	ATOM	1094	1/4	コピパ	A 41	T -3.3T0	23.4/2	43.333	1.00	J4.02	14

-163-

	MOTA	1895	CA	SER		411	-5.611	24.163	30.235	1 00	25 60	_
		1896								1.00		C
	MOTA		C	SER			-5.215	23.008	29.319	1.00		С
	MOTA	1897	0	SER			-4.602	22.040	29.770		35.62	0
_	MOTA	1898	CB	SER .			-7.031	23.928	30.763	1.00		C
5	MOTA	1899	OG	SER .	A	411	-7.959	23.837	29.697	1.00	38.87	0
	MOTA	1900	N	MET	A	412	-5.561	23.108	28.038	1.00	35.70	N
	MOTA	1901	CA	MET .	A	412	-5.244	22.053	27.079		36.25	C
	ATOM	1902	С	MET			-3.744	21.912	26.846		34.53	Č
	ATOM	1903	ō	MET			-3.273	20.867	26.393		34.48	ō
10				MET								
10	ATOM	1904	CB		-		-5.936	22.324	25.741		40.58	C
	ATOM	1905	CG	MET			-7.433	22.563	25.850		45.64	C
	MOTA	1906	SD	MET			-8.214	22.729	24.232	1.00	52.62	S
	MOTA	1907	CE	MET	A	412	-7.402	24.204	23.610	1.00	50.53	C
	ATOM	1908	N	LYS	Α	413	-2.996	22.965	27.150	1.00	31.53	N
15	ATOM	1909	CA	LYS	Α	413	-1.551	22.944	26.960	1.00	30.85	C
	MOTA	1910	C	LYS			-0.831	22.407	28.192		30.52	Č
	ATOM	1911	ō	LYS			0.386	22.236	28.187		30.68	ŏ
		1912										
	ATOM		CB	LYS			-1.042	24.350	26.632		31.05	C
00	ATOM	1913	CG	LYS			-1.557	24.897	25.307		32.36	C
20	MOTA	1914	CD	LYS			-1.030	26.296	25.035		32.77	C
	MOTA	1915	CE	LYS			-1.521	26.812	23.689	1.00	34.50	C
	MOTA	1916	NZ	LYS	Α	413	-3.014	26.878	23.622	1.00	36.17	N
	MOTA	1917	N	LEU	Α	414	-1.590	22.142	29.248	1.00	30.09	N
	ATOM	1918	CA	LEU	Α	414	-1.014	21.620	30.484		28.96	C
25	ATOM	1919	C	LEU			-1.393	20.147	30.610		28.33	Č
	ATOM	1920	Ö	LEU			-1.654	19.489	29.604		29.10	Ö
			-	_	-							
	ATOM	1921	CB	LEU			-1.544	22.427	31.676		28.64	C
	MOTA	1922	CG	LEU			-1.270	23.934	31.581		30.41	С
	ATOM	1923		LEU			-1.967	24.676	32.711	1.00	31.19	C
30	ATOM	1924	CD2				0.226	24.179	31.624	1.00	30.79	C
	ATOM	1925	N	THR	Α	415	-1.401	19.624	31.833	1.00	27.70	N
	MOTA	1926	CA	THR	Α	415	-1.779	18.232	32.071	1.00	26.69	C
	MOTA	1927	С			415	-2.620	18.195	33.338		26.91	C
	MOTA	1928	ō			415	-2.548	19.104	34.157	1.00	26.39	ŏ
35	ATOM	1929	СВ			415	-0.556	17.310	32.307		26.61	c
00			OG1									
	MOTA	1930				415	-0.006	17.570	33.607		25.35	0
	ATOM	1931	CG2				0.509	17.546	31.247		26.48	С
	MOTA	1932	N			416	-3.432	17.142	33.516		27.60	N
	MOTA	1933	CA			416	-4.269	17.037	34.717	1.00	27.16	C
40	ATOM	1934	C	PRO	Α	416	-3.477	17.169	36.026	1.00	27.48	C
	ATOM	1935	0	PRO	Α	416	-3.930	17.813	36.975	1.00	26.90	0
	ATOM	1936	СВ	PRO	Α	416	-4.908	15.661	34.564	1.00	29.00	С
	ATOM	1937	CG			416	-5.083	15.555	33.072		28.36	C
	MOTA	1938	CD			416	-3.752	16.071	32.553		28.22	c
45		1939	N			417	-2.294	16.560	36.072		25.90	
70	ATOM											N
	MOTA	1940	CA			417	-1.460	16.610	37.271		25.39	C
	MOTA	1941	С			417	-0.961	18.031	37.545		24.67	C
	MOTA	1942	0	LEU	A	417	-0.983	18.502	38.685	1.00	24.55	0
	MOTA	1943	CB	LEU	A	417	-0.279	15.643	37.124	1.00	25.12	C
50	MOTA	1944	CG	LEU	Α	417	0.722	15.507	38.273	1.00	25.26	C
	ATOM	1945	CD1	LEU			0.021	15.098	39.564		24.40	С
	ATOM	1946		LEU			1.766	14.470	37.882		25.23	C
	MOTA	1947	N			418	-0.506	18.711	36.500		24.66	N
	ATOM	1948	CA			418	-0.027	20.080	36.640			
55											25.57	C
JJ	MOTA	1949	C			418	-1.176	20.971	37.111		26.33	C
	ATOM	1950	0			418	-1.001	21.814	37.991		27.09	0
	MOTA	1951	CB			418	0.531	20.599	35.297		25.14	C
	MOTA	1952	CG:	L VAL	A	418	0.723	22.112	35.338	1.00	26.89	С

-164-

	MOTA	1953		VAL A		1.861	19.912	35.009	1.00 25.97	C
	MOTA	1954	N	LEU A		-2.354	20.769	36.530	1.00 26.33	N
	MOTA	1955	CA	LEU A		-3.526	21.556	36.902	1.00 27.78	C
_	ATOM	1956	С	LEU A		-3.861	21.399	38.382	1.00 29.03	C
5	ATOM	1957	0	LEU A		-4.206	22.370	39.052	1.00 30.30	0
	MOTA	1958	CB	LEU A		-4.733	21.143	36.051	1.00 28.60	C
	MOTA	1959	CG	LEU A		-4.696	21.585	34.586	1.00 30.69	C
	MOTA	1960		LEU 1		-5.871	20.975	33.828	1.00 30.94	C
40	ATOM	1961		LEU A		-4.743	23.105	34.515	1.00 31.11	С
10	MOTA	1962	N		A 420	-3.738	20.184	38.904	1.00 29.76	N
	ATOM	1963	CA		A 420	-4.056	19.962	40.307	1.00 31.06	C
	ATOM	1964	C		A 420	-3.010	20.514	41.268	1.00 30.59	C
	ATOM	1965	0		A 420	-3.344	21.184	42.245	1.00 30.30	0
45	MOTA	1966	CB		A 420	-4.237	18.478	40.605	1.00 32.62	C
15	ATOM	1967	CG		A 420	-4.697	18.251	42.037	1.00 36.69	C
	MOTA	1968	CD		A 420	-4.267	16.919	42.598	1.00 38.47	C
	MOTA	1969		GLU		-4.631	16.624	43.756	1.00 40.46	0
	MOTA	1970	OE2		A 420	-3.561	16.171	41.891	1.00 41.56	
00	ATOM	1971	N		A 421	-1.744	20.223	40.992	1.00 31.25	
20	MOTA	1972	CA		A 421	-0.663	20.675	41.855	1.00 32.00	
	ATOM	1973	C		A 421	-0.544	22.191	41.960	1.00 32.63	
	ATOM	1974	0		A 421	-0.355	22.724	43.051	1.00 32.82	
	ATOM	1975	CB		A 421	0.694	20.082	41.395	1.00 31.60	
25	ATOM	1976			A 421	1.843	20.676	42.208	1.00 31.31	
25	ATOM	1977			A 421	0.667	18.567	41.556	1.00 31.20	
	ATOM	1978	N		A 422	-0.670	22.890	40.839	1.00 33.47	
	ATOM	1979	CA		A 422	-0.541	24.342	40.857	1.00 34.95	
	ATOM	1980	C		A 422	-1.866	25.089	40.872	1.00 35.99	
20	ATOM	1981	0		A 422	-1.907	26.284	41.159	1.00 36.37	
30	ATOM	1982	CB		A 422	0.310	24.794	39.670	1.00 34.60	
	MOTA	1983	CG		A 422	1.679	24.182	39.656	1.00 34.76	
	MOTA	1984			A 422	2.093	23.389	38.592	1.00 34.88	
	ATOM	1985			A 422	2.545	24.369	40.728	1.00 35.16	
35	ATOM	1986			A 422	3.348	22.790	38.597	1.00 34.92	
33	ATOM	1987	CE2		A 422	3.801	23.774	40.743	1.00 34.70	
	MOTA	1988	CZ		A 422	4.202	22.982 24.378	39.674 40.570	1.00 34.73	
	MOTA	1989 1990	N		A 423	-2.946	24.376	40.570	1.00 37.39	
	MOTA		CA C		A 423	-4.261 -4.914	24.993	41.930	1.00 38.8	
40	ATOM	1991	0		A 423 A 423	-5.857	24.907	42.083	1.00 39.70	
40	ATOM TER	1992 1993	U		A 423	-5.657	24.033	42.003	1.00 40.5	. 0
	HETATM		02		425	17.029	18.071	3/ 810	1.00 21.73	3 0
	HETATM		03	VDX	425	4.489	26.946	35.054	1.00 24.6	
	HETATM		C1	VDX	425	14.139	17.953	35.755	1.00 20.80	
45	HETATM		C2	VDX	425	14.879	16.893	34.895	1.00 21.0	
70	HETATM		C3	VDX	425	15.992	17.534	33.962	1.00 21.4	
	HETATM		C4	VDX	425	15.368	18.672	33.049	1.00 21.2	
	HETATI		C5	VDX	425	14.622		33.864		
	HETATI		C6	VDX	425	14.797		33.792	1.00 20.9	
50	HETATI		C7	VDX	425	14.174		34.514		
00	HETATI		C8	VDX	425	13.966		34.042	1.00 21.5	
		1 2004	C9	VDX	425	14.354		32.544		
		1 2004		VDX	425	13.602		34.828		
		4 2005 4 2006		1 VDX				31.671		
55		M 2000 M 2007		2 VDX				32.564		
50		M 2007		3 VDX						
		м 2009 м 2009		4 VDX						
		M 2010		5 VDX						
			~							. •

-165-

	HETATM	2011	C16	VDX	425	11.429	25.231	36.497	1.00	22.39	C
	HETATM	2012	C17	VDX	425	11.276	25.934	35.106	1.00	22.31	С
	HETATM	2013	C18	VDX	425	10.769	23.570	33.779	1.00	21.50	С
	HETATM	2014	C19	VDX	425	12.291	19.455	34.852	1.00	20.77	С
5	HETATM	2015	C20	VDX	425	9.849	26.546	34.726	1.00	22.90	C
	HETATM	2016	C21	VDX	425	9.804	27.956	35.482	1.00	23.65	C
	HETATM	2017	C22	VDX	425	8.575	25.824	35.268	1.00	23.16	С
	HETATM	2018	C23	VDX	425	7.331	26.060	34.405	1.00	23.73	C
	HETATM	2019	C24	VDX	425	6.152	25.266	34.672	1.00	24.36	C
10	HETATM	2020	C25	VDX	425	4.775	25.776	34.336	1.00	24.75	С
	HETATM	2021	C26	VDX	425	4.701	26.010	32.842	1.00	25.41	C
	HETATM	2022	C27	VDX	425	3.668	24.730	34.723	1.00	25.39	С
	HETATM	2023	01	VDX	425	13.119	17.359	36.620	1.00	20.68	0
	HETATM	2024	0	HOH	500	14.347	10.333	30.796	1.00	24.33	0
15	HETATM	2025	0	HOH	501	13.828	12.782	35.922	1.00	21.46	0
	HETATM	2026	0	нон	502	13.846	14.468	42.856	1.00	24.78	0
	HETATM	2027	0	нон	503	19.132	15.890	40.266	1.00	21.27	0
	HETATM	2028	0	HOH	504	15.013	12.029	41.977	1.00	22.69	0
	HETATM	2029	O	HOH	505	13.766	10.118	35.125	1.00	20.29	0
20	HETATM	2030	0	HOH	506	16.290	13.157	34.345	1.00	30.57	0
	HETATM	2031	0	HOH	507	5.938	22.747	23.179	1.00	24.25	0
	HETATM	2032	0	HOH	508	13.771	7.592	35.963	1.00	28.23	0
	HETATM		0	HOH	509	12.348	25.386	50.763	1.00	30.93	0
	HETATM	2034	0	HOH	510	28.498	23.703	34.824	1.00	37.09	0
25	HETATM	2035	0	HOH	511	26.394	10.521	64.086	1.00	30.68	0
	HETATM	2036	0	HOH	512	20.573	9.150	38.613	1.00	30.36	0
	HETATM	2037	0	HOH	513	19.724	30.629	29.203	1.00	35.40	0
	HETATM	2038	0	HOH	514	4.372	27.504	42.595	1.00	31.46	0
	HETATM	2039	0	HOH	515	2.808	13.423	33.286	1.00	30.93	0
30	HETATM	2040	0	HOH	516	23.698	20.154	43.135		37.92	0
	HETATM	2041	0	HOH	517	11.325	5.901	37.588	1.00	30.12	0
	HETATM		0	HOH	518	0.885	13.049	59.537	1.00	39.32	0
	HETATM	2043	0	HOH	519	20.338	11.515	62.065	1.00	36.13	0
	HETATM		0	HOH	520	8.913	6.134	53.451		44.37	0
35	HETATM		0	HOH	521	4.924	23.321	44.129		33.51	0
	HETATM		0	HOH	522	16.547	6.409	36.375		32.70	0
	HETATM		0	HOH	523	8.896	35.918	45.789		45.73	0
	HETATM		0	нон	524	26.192	21.542	43.420		28.56	0
40	HETATM		0	нон	525	-5.345	32.214	23.915		35.31	0
40	HETATM		0	HOH	526	9.488	15.901	22.976		29.33	0
	HETATM		0	нон	527	5.345	31.465	22.796		31.37	0
	HETATM		0	нон	528						0
	HETATM		0	нон	529	4.642	13.886	30.953		31.71	0
AF	HETATM		0	нон	530	-3.764	29.115	25.550		37.63	0
45	HETATM		0	нон	531	31.831	9.097	66.550		36.20	0
	HETATM		0	HOH	532	10.178	6.595	32.965		30.94	0
	HETATM		0	нон	533	-1.561	14.197	34.245		33.20	0
	HETATN		0	нон	534	0.476	12.154	62.160		39.93	0
EΛ	HETATN		0	нон	535	25.970	5.142	53.011		47.31	0
50	HETATN		0	нон	536	8.695	5.045	44.801		38.39	0
	HETATI		0	нон	537	22.396	11.047	39.112		40.45	0
	HETATI		0	НОН	538	13.975	29.983	22.553		36.21	0
	HETATI		0	нон	539	-6.673	18.195	37.122		36.41	0
EE	HETATI		0	нон	540	15.926	27.813	55.197		43.43	0
55	HETATI		0	НОН	541	21.922	29.786	26.625		39.42	0
	HETATI		0	НОН	542	29.079	22.924	57.335		43.49	0
	HETATI			нон	543	-8.883	26.986			47.42	0
	HETAT	1 2068	0	нон	544	-2.789	31.232	23.837	1.00	38.14	0

-166-

	HETATM	2069	0	нон	545	15.578	33.329	45.128	1.00 3	9.44	0
	HETATM	2070	0	нон	546	20.810	2.660	42.920	1.00 5	1.44	0
	HETATM	2071	0	HOH	547	27.448	25.982	58.310	1.00 4	13.04	0
	HETATM	2072	0	HOH	548	21.987	8.152	64.287	1.00 4	13.15	0
5	HETATM	2073	0	нон	549	14.435	13.091	64.840	1.00 3	35.87	0
	HETATM		Ō	НОН	550	1.276	25.772	21.944	1.00 4		0
	HETATM		ŏ	нон	551	14.102	6.513	31.763	1.00 4		ō
	HETATM		ō	нон	552	11.990	24.017	53.147	1.00 4		ŏ
	HETATM		ŏ	нон	553	3.481	24.236	20.666	1.00		ŏ
10	HETATM		ŏ	нон	55 4	24.054	13.110	35.770	1.00		ŏ
	HETATM		Ö	нон	556	6.857	37.182	44.351	1.00		Ö
			-		557	-8.644	30.901		1.00		
	HETATM		0	нон			33.571	30.925 43.159			0
	HETATM		0	нон	558	17.767			1.00		0
45	HETATM		0	нон	559	16.954	26.537	23.238	1.00 9		0
15	HETATM		0	нон	560	27.386	20.638	40.959	1.00		0
	HETATM		0	нон	561	31.418	10.182	50.496	1.00		0
	HETATM		0	нон	562	4.082	21.082	20.610	1.00		0
	HETATM		0	нон	563	14.064	10.706	58.224	1.00		0
	HETATM		0	HOH	564	23.415	29.835	49.803	1.00		0
20	HETATM		0	HOH	565	14.533	11.393	24.395	1.00		0
	HETATM	2089	0	HOH	566	-0.868	36.798	40.025	1.00	52.17	0
	HETATM	2090	0	HOH	567	2.865	34.386	33.570	1.00	42.56	0
	HETATM	2091	0	HOH	568	-4.893	19.288	30.751	1.00	44.30	0
	HETATM	2092	0	HOH	569	30.643	14.674	61.949	1.00	43.28	0
25	HETATM	2093	0	HOH	570	22.702	3.372	47.417	1.00	36.93	0
	HETATM	2094	0	нон	571	13.379	35.172	44.109	1.00	47.38	0
	HETATM	2095	0	HOH	572	-1.138	20.698	22.966	1.00	53.61	0
	HETATM		0	нон	573	25.589	19.849	33.401		52.13	0
	HETATM		Ŏ	нон	574	23.893	13.360	32.579		45.26	Ō
30	HETATM		ō	нон	575	-7.367	18.485	31.944		48.23	ō
-	HETATM		ō	нон	576	2.430	19.200	65.790		45.13	ŏ
	HETATM		ŏ	нон	577	20.048	32.028	44.907		46.82	ŏ
	HETATM			нон	578	20.286	6.713	37.519		43.08	ŏ
	HETATM			нон	579	25.879	5.448	50.403		48.82	ŏ
35	HETATM			нон	580	24.905	19.763	39.659		45.39	o
00	HETATM			нон	581	2.341	14.233	26.082		50.76	o
	HETATM			нон нон	582	15.248	20.000	60.506		44.08	0
								37.715			
	HETATM			НОН	583	22.695	7.038			46.55	0
40	HETATM			НОН	584	11.915	16.625	66.479		52.58 46.90	0
40	HETATM			нон	585	20.145	35.730	35.936			0
	HETATM		_	нон	586	10.735	24.933	16.684		46.64	0
	HETATM			нон	587	1.182	9.495	61.830		55.88	0
	HETATM			нон	588	-3.993	16.527	51.745		43.33	0
AE	HETATM			нон	589	21.842	29.919	56.624		42.17	0
45	HETATM			нон	590	3.602	25.520	44.494		50.24	0
	HETATM			НОН	591	1.198	23.984	44.777		43.76	0
	HETATM			НОН	592	13.208	27.713	54.123		59.17	0
	HETATM			нон	593	27.958	7.530	50.434		53.55	0
	HETATM			нон	594	22.594	3.510	64.140		45.66	0
50	HETATM			HOH	595	30.412	22.979	36.623		71.37	0
	HETATN			HOH	596	10.560	15.906	20.574		50.32	0
	HETATN			HOH	597	26.021	3.241	64.667		49.85	0
	HETATI	1 2121	. 0	НОН	598	19.853	9.062	62.967	1.00	56.45	0
	HETATI	1 2122	. 0	нон	599	12.462	3.992	52.363	1.00	42.46	0
55	HETATI	4 2123	0	НОН	600	6.152	35.657	28.721	1.00	46.87	0
	HETATI			нон	601	7.626	29.983	53.085		51.73	0
	HETATI			нон	602	11.547	23.591	57.064		51.07	ō
	HETATI			нон	603	24.407	19.393	31.035		53.85	ŏ

-167-

	HETATM		0	нон	604	12.538	23.006	18.706	1.00		0
	HETATM		0	нон	605	1.839	16.469	66.997	1.00 4		0
	HETATM		0	НОН	606	1.378	19.964	21.070	1.00 4		0
_	HETATM		0	HOH	607	5.895	26.935	51.419	1.00		0
5	HETATM		0	нон	608	13.122	33.698	19.464	1.00		0
	HETATM		0	нон	609	27.040	8.636	44.102	1.00		0
	HETATM		0	HOH	610	18.833	30.775	55.879	1.00		0
	HETATM	2134	0	HOH	611	34.509	17.720	47.771	1.00		0
	HETATM		0	нон	612	18.356	32.644	25.579	1.00		0
10	HETATM	2136	0	HOH	613	-2.259	16.235	28.804	1.00		0
	HETATM	2137	0	HOH	614	16.400	38.404	21.700	1.00		0
	HETATM	2138	0	HOH	615	9.340	39.540	19.060	1.00		0
	HETATM	2139	0	HOH	616	20.026	35.074	32.855	1.00		0
	HETATM		0	HOH	617	31.604	8.486	59.428	1.00		0
15	HETATM	2141	0	HOH	618	26.228	8.975	40.708	1.00		0
	HETATM	2142	0	HOH	619	0.460	15.378	28.064	1.00	50.21	0
	HETATM	2143	0	НОН	620	15.771	3.385	48.139	1.00	38.09	0
	HETATM	2144	0	HOH	621	25.135	17.914	42.644	1.00	60.05	0
	HETATM	2145	0	HOH	622	-2.286	29.197	21.618	1.00	53.99	0
20	HETATM	2146	0	HOH	623	32.865	18.926	45.658	1.00	48.11	0
	HETATM	2147	0	HOH	624	17.116	13.333	25.240	1.00	52.60	0
	HETATM	2148	0	HOH	625	-2.809	17.978	56.255	1.00	53.36	0
	HETATM	2149	0	нон	626	-3.647	7.885	56.347	1.00	63.91	0
	HETATM	2150	0	HOH	627	17.746	24.596	21.608	1.00	59.81	0
25	HETATM	2151	0	HOH	628	28.368	5.841	47.861	1.00	66.08	0
	HETATM	2152	0	HOH	629	13.641	11.618	66.858	1.00	52.02	0
	HETATM	2153	0	HOH	630	8.052	20.893	16.742	1.00	53.91	0
	HETATM	2154	0	HOH	631	8.914	38.015	27.578	1.00	56.47	0
	HETATM		0	нон	632	9.081	13.482	19.627	1.00	57.14	0
30	HETATM		0	нон	633	-4.343	24.969	37.694	1.00	51.08	0
	HETATM	2157	0	HOH	634	3.597	28.859	46.576	1.00	54.80	0
	HETATM	2158	0	HOH	635	27.905	21.432	28.373	1.00	59.49	0
	HETATM	2159	0	HOH	636	-4.252	18.337	25.491	1.00	47.50	0
	HETATM	2160	0	HOH	637	-2.808	23.046	51.839	1.00	49.04	0
35	HETATM	2161	0	HOH	638	2.757	25.756	18.437	1.00	49.80	0
	HETATM	2162	0	HOH	639	15.470	7.390	63.803	1.00	52.42	0
	HETATM	2163	0	HOH	640	33.689	11.757	50.784	1.00	54.00	0
	HETATM	2164	0	HOH	641	6.223	13.352	20.927	1.00	49.77	0
	HETATM	2165	0	HOH	642	12.267	32.764	51.605	1.00	48.76	0
40	HETATM	2166	0	HOH	644	25.211	3.585	48.391	1.00	49.75	0
	HETATM	2167	0	нон	645	0.619	24.002	51.358	1.00	49.46	0
	HETATM	2168	0	HOH	646	12.270	22.627	60.617	1.00	63.88	0
	HETATM	2169	0	HOH	647	0.202	23.805	47.834	1.00	52.54	0
	HETATM	1 2170	0	HOH	648	15.471	8.169	23.816	1.00	54.49	0
45	HETATM	1 2171	. 0	HOH	649	4.098	13.117	28.105	1.00	43.97	0
	HETATM	1 2172	0	HOH	650	16.032	4.857	59.064	1.00	55.67	0
	HETATM			HOH	651	-5.591	11.911	55.960	1.00	63.35	0
	HETATM			HOH	652	14.373	4.083	36.218	1.00	49.18	0
	HETATM			нон	653	11.138	5.501	59.825	1.00	51.19	0
50	HETATM			нон	654	26.262	1.299	50.288	1.00	61.20	0
	HETATM			нон	655	4.067	20.751	67.111	1.00	51.75	0
	HETATM			нон	656	11.291		23.646		53.35	0
	HETATN			нон	657	2.505		45.342		58.29	0
	HETATI			нон	658	18.881				60.82	0
55	HETATI			нон	659	-1.930				65.05	0
	HETATI			нон	660	-3.587				51.24	
	HETATI			нон	661					58.94	
	HETATI			нон	662					60.06	
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-168-

HETATM	2185	0	НОН	663	30.991	26.420	51.105	1.00 54.69	0
HETATM	2186	0	HOH	664	16.115	30.354	56.207	1.00 60.96	0
HETATM	2187	0	нон	665	36.596	19.242	55.988	1.00 55.83	0

-169-

Table 3 Atomic Structure Coordinate Data of Polyalanine Model of Conserved VDR LBD

5									_		
	MOTA	1	СВ	PRO	103	-17.052			1.00 78.63	A	C
	MOTA	2	CG	PRO	103	-16.933			1.00 78.57	Α	С
	MOTA	3	C	PRO	103	-15.322			1.00 78.42	Α	С
	ATOM	4	0	PRO	103	-15.845			1.00 78.37	A	0
10	MOTA	5	N	PRO	103		-27.870		1.00 78.63	A	N
	MOTA	6	CD	PRO	103		-28.350		1.00 78.61	A	С
	MOTA	7	CA	PRO	103		-26.943		1.00 78.57	A	C
	MOTA	8	N	VAL	104		-25.636		1.00 78.14	A	N
	MOTA	9	CA	VAL	104		-24.422		1.00 77.74	A	C
15	MOTA	10	CB	VAL	104		-24.729		1.00 77.77	A	C
	MOTA	11		VAL	104		-25.415		1.00 77.66	Α	С
	ATOM	12		VAL	104		-25.591		1.00 77.68	A	C
	MOTA	13	С	VAL	104	-14.153	-23.671	136.828	1.00 77.43	A	С
	ATOM	14	0	VAL	104		-24.202		1.00 77.67	A	0
20	MOTA	15	N	GLN	105	-13.726	-22.427	136.636	1.00 76.69	Α	N
	MOTA	16	CA	GLN	105	-14.254	-21.567	135.582	1.00 75.70	A	C
	MOTA	17	CB	GLN	105	-13.976	-20.099	135.918	1.00 76.09	Α	C
	ATOM	18	CG	GLN	105	-12.491	-19.779	136.067	1.00 76.08	Α	C
	ATOM	19	CD	GLN	105	-12.210	-18.291	136.099	1.00 76.03	Α	С
25	MOTA	20	OE1		105			135.107	1.00 75.85	Α	0
	MOTA	21	NE2	GLN	105	-11.739	-17.800	137.241	1.00 75.74	Α	N
	MOTA	22	С	GLN	105	-13.637	-21.877	134.223	1.00 74.59	Α	C
	MOTA	23	0	GLN	105	-12.719	-22.691	134.111	1.00 74.90	A	0
	ATOM	24	N	LEU	106			133.193	1.00 72.98	Α	N
30	ATOM	25	CA	LEU	106	-13.654	-21.381	131.836	1.00 71.07	A	C
	ATOM	26	CB	LEU	106			131.032	1.00 71.27	Α	С
	MOTA	27	CG	LEU	106			129.638	1.00 71.35	Α	C
	ATOM	28		LEU	106			129.733	1.00 71.22	A	С
	ATOM	29		LEU	106			129.027	1.00 71.16	Α	С
35	MOTA	30	C	LEU	106	-13.537	-20.002	131.185	1.00 69.48	Α	C
	ATOM	31	0	LEU	106	-14.517	-19.447	130.693	1.00 69.41	Α	0
	MOTA	32	N	SER	107			131.211	1.00 67.67		N
	ATOM	33	CA	SER	107	-12.021	-18.145	130.645	1.00 65.85	Α	С
	MOTA	34	CB	SER	107			130.383	1.00 65.62	Α	C
40	MOTA	35	QG	SER	107			129.625	1.00 65.53		0
	ATOM	36	С	SER	107			129.360	1.00 64.86		C
	ATOM	37	0	SER	107			128.573	1.00 64.79		0
	ATOM	38	N	LYS	108			129.154	1.00 63.49		N
4=	ATOM	39	CA	LYS	108			127.948	1.00 62.43		C
45	ATOM	40	СВ	LYS	108			128.055	1.00 62.56		C
	ATOM	41	CG	LYS	108			128.417	1.00 62.85		C
	ATOM	42	CD	LYS	108			129.776	1.00 63.11		C
	MOTA	43	CE	LYS	108			130.129	1.00 63.62		C
	MOTA	44	NZ	LYS	108			131.449	1.00 63.58		N
50	ATOM	45	C	LYS	108			126.750	1.00 61.42		C
	MOTA	46	0	LYS	108			125.661	1.00 61.44		0
	MOTA	47	N	GLU	109			126.959	1.00 60.15		N
	ATOM	48	CA	GLU	109			125.900	1.00 58.91		C
	ATOM	49	CB	GLU	109			126.358	1.00 59.90		_
55	MOTA	50	CG	GLU	109	-8.171	-15.661	125.279	1.00 61.96	A	С

-170-

	MOTA	51	CD GLU	109			125.745	1.00 63.27		C
	MOTA	52	OE1 GLU	109			126.160	1.00 64.16		0
	MOTA	53	OE2 GLU	109			125.696	1.00 63.84		0
_	MOTA	54	C GLU	109	-10.443			1.00 57.30		C
5	MOTA	55	O GLU	109	-10.154			1.00 56.66	A	0
	MOTA	56	N GLN	110	-10.655			1.00 55.60	A	N
	MOTA	57	CA GLN	110	-10.564			1.00 54.48	A	C
	MOTA	58	CB GLN	110	-10.456			1.00 53.38	A	C
40	MOTA	59	CG GLN	110			128.310	1.00 52.62	A	C
10	ATOM	60	CD GLN	110			129.642	1.00 52.04	A	C
	ATOM	61	OE1 GLN		-7.901	-21.441		1.00 51.99	A	N O
	MOTA	62	NE2 GLN				125.503	1.00 51.70 1.00 54.10	A	C
	ATOM	63	C GLN				124.671	1.00 54.10	A A	0
15	MOTA	64 65	O GLN N GLU				125.772	1.00 53.77	A	N
13	ATOM ATOM	66	CA GLU				125.772	1.00 53.80	A	C
	ATOM	67	CB GLU				125.774	1.00 54.85	A	c
	ATOM	68	CG GLU				127.131	1.00 56.90	A	c
	MOTA	69	CD GLU				127.793	1.00 58.68	A	c
20	ATOM	70	OE1 GLU				127.171	1.00 60.00	A	ŏ
20	MOTA	71	OE2 GLU				128.936	1.00 59.57	A	ŏ
	ATOM	72	C GLU				123.610	1.00 52.44	Α	Ċ
	ATOM	73	O GLU				122.747	1.00 52.44	A	ō
	ATOM	74	N GLU				123.334	1.00 50.93	A	N
25	ATOM	75	CA GLU				121.968	1.00 49.46	A	C
	ATOM	76	CB GLU				121.956	1.00 50.56	A	C
	ATOM	77	CG GLU		-14.044	-16.030	121.322	1.00 52.74	Α	C
	MOTA	78	CD GLU		-15.427	-16.308	121.887	1.00 53.94	A	С
	ATOM	79	OE1 GLU	J 112	-15.634	-16.105	123.106	1.00 54.84	Α	0
30	ATOM	80	OE2 GLU	112	-16.306	-16.737	121.110	1.00 54.87	Α	0
	ATOM	81	C GLU	112	-12.332	-19.204	121.212	1.00 47.53	Α	C
	ATOM	82	O GL	J 112	-12.470	-19.442	120.015	1.00 47.52	A	0
	MOTA	83	N LE	J 113	-11.290	-19.622	2 121.922	1.00 45.16	A	N
	ATOM	84	CA LE				121.341	1.00 42.62	Α	C
35	ATOM	85	CB LE				2 122.418	1.00 42.09	A	C
	MOTA	86	CG LE				122.021	1.00 42.04	A	С
	MOTA	87	CD1 LE				123.223	1.00 41.08	A	C
	ATOM	88	CD2 LE				120.836	1.00 41.07	A	C
40	MOTA	89	C LE				120.824	1.00 41.07	A	С
40	MOTA	90	O LE				5 119.670	1.00 39.68	A	0
	MOTA	91	N IL				7 121.706	1.00 39.49	A	N
	MOTA	92	CA IL				3 121.395	1.00 39.05 1.00 37.48		C
	MOTA	93	CB IL				2 122.660 3 122.313	1.00 37.48	A A	C
45	MOTA	94	CG2 IL				9 123.709	1.00 37.03	A	C
73	MOTA	95 96					7 125.034	1.00 35.81	A	C
	ATOM ATOM	97	C IL				2 120.267	1.00 39.39	A	
	ATOM	98					0 119.440	1.00 39.39	A	ō
	MOTA	99					0 120.229	1.00 39.79	A	N
50	ATOM	100					3 119.185		A	
•	ATOM	101					B 119.473		A	
	ATOM	102					8 118.451		A	
	ATOM	103					2 118.113		Α	
	ATOM	104					6 117.470		A	
55	ATOM	105					6 117.053		Α	
	ATOM	106					3 117.207		A	
	MOTA	107		G 115	-14.100	-16.89	9 116.478	1.00 53.49	Α	N
	MOTA	108	C AR	G 115	-14.327	7 -21.82	4 117.839	1.00 39.30	Α	С

-171-

	ATOM	109	0	ARG	115	-14.794	-22.357	116.833	1.00 39.26	A	0
	ATOM	110	N	THR	116	-13.190			1.00 37.95		N
	ATOM	111	CA	THR	116	-12.389		116.626	1.00 36.97		С
	ATOM	112	СВ	THR	116	-11.177		116.900	1.00 37.51		С
5	ATOM	113	0G1	THR	116		-18.847		1.00 39.12		0
•	ATOM	114	CG2	THR	116	-10.434			1.00 37.41		С
	ATOM	115	C	THR	116	-11.887		116.122	1.00 35.58		C
	ATOM	116	Ö	THR	116	-11.905		114.921	1.00 35.61	Α	0
	MOTA	117	N	LEU	117	-11.434			1.00 33.47	A	N
10	MOTA	118	CA	LEU	117	-10.932			1.00 31.78	A	C
. •	ATOM	119	CB	LEU	117	-10.286			1.00 30.67	A	C
	ATOM	120	CG	LEU	117		-24.582		1.00 30.04	A	C
	ATOM	121		LEU	117				1.00 29.00	A	C
	ATOM	122		LEU	117		-24.735		1.00 30.20	Α	С
15	ATOM	123	C	LEU	117		-25.413		1.00 31.49	A	С
. •	ATOM	124	Ö	LEU	117		-26.112		1.00 31.28	A	0
	ATOM	125	N	LEU	118		-25.413		1.00 31.24	A	N
	ATOM	126	CA	LEU	118		-26.233		1.00 30.90	A	С
	MOTA	127	СВ	LEU	118			117.510	1.00 30.93	A	C
20	MOTA	128	CG	LEU	118		-26.707		1.00 31.21	A	C
	ATOM	129		LEU	118		-26.391		1.00 31.43	A	C
	MOTA	130		LEU	118			118.737	1.00 30.10	A	C
	ATOM	131	C	LEU	118			115.111	1.00 30.73	A	С
	ATOM	132	ŏ	LEU	118			114.287	1.00 30.25	Α	0
25	ATOM	133	N	GLY	119			114.872	1.00 30.45	A	N
	ATOM	134	CA	GLY	119			113.586	1.00 29.84	A	C
	ATOM	135	C	GLY	119	-14.551	-24.519	112.445	1.00 29.41	Α	С
	ATOM	136	Ö	GLY	119	-15.036	-24.986	111.411	1.00 29.26	A	0
	ATOM	137	N	ALA	120			112.634	1.00 28.27	Α	N
30	MOTA	138	CA	ALA	120			111.623	1.00 27.50	A	C
_	MOTA	139	СВ	ALA	120			112:006	1.00 28.11	A	C
	ATOM	140	C	ALA	120	-12.273	-26.317	111.455	1.00 26.73	Α	С
	ATOM	141	0	ALA	120	-12.223	-26.826	110.336	1.00 26.07	A	0
	MOTA	142	N	HIS	121	-12.348	-27.038	112.569	1.00 26.34	Α	N
35	MOTA	143	CA	HIS	121	-12.356	-28.498	112.542	1.00 25.51	Α	C
	MOTA	144	СВ	HIS	121	-12.250	-29.053	113.967	1.00 25.42	A	C
	MOTA	145	CG	HIS	121	-12.478	-30.531	114.058	1.00 25.78	A	С
	ATOM	146		2 HIS	121	-11.622	-31.573	113.949	1.00 25.53	Α	C
	ATOM	147		1 HIS	121	-13.729	-31.082	114.240	1.00 26.55	A	N
40	ATOM	148	CE	1 HIS	121	-13.633	-32.398	114.239	1.00 27.01	Α	C
	ATOM	149	NE:	2 HIS	121			114.064	1.00 27.07	Α	N
	MOTA	150	C	HIS	121			111.857	1.00 25.65	Α	C
	MOTA	151	. 0	HIS	121			111.000	1.00 23.32	A	0
	ATOM	152	N	THR	122			2 112.233	1.00 26.18	A	N
45	MOTA	153	CA	THR	122			1 111.644	1.00 27.73	Α	C
	ATOM	154	CB	THR	122			L 112.310	1.00 27.99	Α	C
	ATOM	155	o o o o o	1 THR	122			112.194	1.00 32.40	Α	0
	MOTA	156	G CG	2 THR	122			113.780		Α	С
	ATOM	157	7 C	THR	122			9 110.137	1.00 27.54	Α	С
50	ATOM	158	3 0	THR	122		29.65			Α	0
	ATOM	159	N	ARG	123		3 -27.62			A	N
	MOTA	160		ARG	123	-15.612		9 108.300		Α	С
	MOTA	161	L CB	ARG				2 108.141		A	_
_	ATOM	162						6 106.727		A	
55	MOTA	163	3 CE	ARG				5 106.536		Α	_
	MOTA	164	4 NE					3 107.179		Α	
	MOTA	169						1 106.714		A	_
	MOTA	160	6 NH	11 ARG	123	-17.71	5 -22.88	8 105.592	1.00 37.38	A	N

-172-

	ATOM	167	NH2	ARG	123	-17.913	-21.458	107.366	1.00 37.20	A	N
	MOTA	168	С	ARG	123	-14.628	-28.055	107.415	1.00 28.35	Α	С
	ATOM	169	0	ARG	123	-14.967	-28.431	106.290	1.00 27.61	A	0
	ATOM	170	N	HIS	124	-13.426	-28.324	107.923	1.00 27.75	Α	N
5	ATOM	171	CA	HIS	124	-12.409	-29.016	107.125	1.00 27.66	A	С
	ATOM	172	CB	HIS	124	-11.148	-28.147	107.062	1.00 28.26	A	C
	ATOM	173	CG	HIS	124	-11.395			1.00 29.25	A	С
	ATOM	174	CD2		124	-11.945			1.00 28.40	Α	C
	ATOM	175	ND1		124		-25.631		1.00 29.27	A	N
10	ATOM	176	CE1		124			106.567	1.00 28.76	A	C
	ATOM	177	NE2	_	124		-24.960		1.00 29.33	A	N
	ATOM	178	C	HIS	124			107.478	1.00 26.91	A	C
	ATOM	179	ō	HIS	124			106.599	1.00 26.66	A	Ō
	ATOM	180	N	MET	125			108.735	1.00 26.01	A	N
15	ATOM	181	CA	MET	125			109.108	1.00 26.25	A	C
	ATOM	182	CB	MET	125			110.025	1.00 26.44	A	Ċ
	MOTA	183	CG	MET	125			109.424	1.00 27.40	A	c
	MOTA	184	SD	MET	125			110.350	1.00 31.87	A	s
	ATOM	185	CE	MET	125			111.998	1.00 31.61	A	c
20	ATOM	186	c	MET	125			109.731	1.00 25.47	A	Č
	ATOM	187	ŏ	MET	125			109.446	1.00 25.35	A	ō
	ATOM	188	N	GLY	126			110.581	1.00 24.84	A	N
	ATOM	189	CA	GLY	126			111.247	1.00 24.24	A	c
	ATOM	190	C	GLY	126			110.426	1.00 23.67	A	Č
25	ATOM	191	Ö	GLY	126			110.883	1.00 23.66	A	ō
	ATOM	192	N	THR	127			109.215	1.00 22.39	A	N
	ATOM	193	CA	THR	127			108.390	1.00 22.17	A	C
	ATOM	194	CB	THR	127			108.101	1.00 21.86	A	Č
	ATOM	195	OG1		127			107.497	1.00 21.82	A	Ö
30	MOTA	196	CG2		127			109.387	1.00 22.67	A	Ċ
	ATOM	197	C	THR	127			107.067	1.00 21.87	A	C
	ATOM	198	ō	THR	127			106.118	1.00 21.50	A	ō
	ATOM	199	N	MET	128			106.996	1.00 21.50	A	N
	ATOM	200	CA	MET	128			105.746	1.00 21.52	A	C
35	ATOM	201	СВ	MET	128			105.845	1.00 22.11	A	C
	ATOM	202	CG	MET	128			106.770	1.00 22.14	A	Č
	ATOM	203	SD	MET	128		-34.750		1.00 21.82	A	s
	ATOM	204	CE	MET	128			108.065	1.00 22.47	A	C
	ATOM	205	C	MET	128			105.315	1.00 21.38	A	C
40	ATOM	206	O	MET	128			104.131	1.00 21.52	Α	0
	ATOM	207	N	PHE	129			106.265	1.00 21.94	Α	N
	ATOM	208	CA	PHE	129	-13.399	-39.231	105.939	1.00 21.94	A	C
	ATOM	209	СВ	PHE	129	-13.509	-40.080	107.219	1.00 21.34	Α	C
	ATOM	210	CG	PHE	129	-14.896	-40.130	107.811	1.00 21.67	Α	С
45	ATOM	211		PHE	129	-15.849	-41.026	107.322	1.00 21.16	Α	С
	ATOM	212		PHE	129			108.855	1.00 20.50	Α	С
	ATOM	213		PHE	129	-17.137	-41.077	107.869	1.00 21.61	A	С
	ATOM	214	CE2		129	-16.533	-39.327	109.406	1.00 21.65	A	С
	ATOM	215	CZ	PHE	129	-17.477	-40.225	108.912	1.00 21.57	Α	C
50	ATOM	216	С	PHE	129	-14.484	-39.644	104.938	1.00 21.50	A	С
	ATOM	217	0	PHE	129	-14.315	-40.613	3 104.197	1.00 20.88	A	0
	ATOM	218	N	GLU	130	-15.589	-38.906	5 104.911	1.00 21.77	Α	N
	ATOM	219	CA	GLU	130			7 103.996	1.00 23.20	Α	С
	ATOM	220	СВ	GLU	130			7 104.298	1.00 23.75	Α	С
55	ATOM	221	CG	GLU	130	-18.476	-38.533	3 105.681	1.00 26.72	Α	C
	ATOM	222	CD	GLU	130	-19.666	-37.630	105.968	1.00 27.23	Α	С
	ATOM	223		L GLU	130			l 105.154		Α	
	ATOM	224		GLU	130	-20.321	37.83	107.014	1.00 28.12	Α	

-173-

	ATOM	225	С	GLU	130	-16.313	-39.072	102.519	1.00 22.81	A	С
	ATOM	226	0	GLU	130	-17.020	-39.581	101.648	1.00 22.98	A	0
	ATOM	227	N	GLN	131	-15.211	-38.396	102.225	1.00 22.34	Α	N
Ω	ATOM	228	CA	GLN	131		-38.251		1.00 23.67	A	C
5	ATOM	229	CB	GLN	131	-14.212	-36.864	100.579	1.00 25.71	A	C
	MOTA	230	CG	GLN	131	-14.915	-35.665	101.279	1.00 31.91	A	С
	ATOM	231	CD	GLN	131	-16.421	-35.495	100.986	1.00 35.53	A	C
	MOTA	232	OE1	GLN	131	-17.020	-34.490	101.382	1.00 39.09	A	0
	MOTA	233	NE2	GLN	131		-36.465		1.00 37.15	A	N
10	MOTA	234	С	GLN	131		-39.344	100.350	1.00 22.82	A	С
	ATOM	235	0	GLN	131		-39.350	99.186	1.00 22.74	A	0
	MOTA	236	N	PHE	132		-40.274		1.00 21.59	A	N
	MOTA	237	CA	PHE	132	-12.585	-41.345	100.840	1.00 20.93	A	C
	ATOM	238	CB	PHE	132	-12.287	-42.289	102.023	1.00 19.90	A	C
15	MOTA	239	CG	PHE	132	-11.445	-41.667	103.133	1.00 19.86	Α	С
	MOTA	240	CD1	PHE	132	-10.858	-40.409	102.982	1.00 19.07	Α	C
	MOTA	241	CD2	PHE	132	-11.258	-42.347	104.337	1.00 18.20	A	C
	MOTA	242	CE1	PHE	132	-10.104	-39.834	104.010	1.00 18.72	A	C
	MOTA	243	CE2	PHE	132	-10.507	-41.783	105.371	1.00 18.68	A	C
20	ATOM	244	CZ	PHE	132	-9.928	-40.525	105.211	1.00 18.24	A	C
	MOTA	245	С	PHE	132		-42.169		1.00 20.71	Α	C
	ATOM	246	0	PHE	132	-12.330	-42.675	98.861	1.00 20.20	A	0
	MOTA	247	N	VAL	133	-14.442	-42.300	99.538	1.00 20.69	A	N
0=	ATOM	248	CA	VAL	133	-15.034	-43.076	98.438	1.00 22.08	A	C
25	MOTA	249	CB	VAL	133	-16.554	-43.305	98.625	1.00 22.06	A	C
	ATOM	250		VAL	133		-44.205		1.00 22.30	A	C
	MOTA	251		VAL	133		-41.975		1.00 20.84	Α	C
	ATOM	252	C	VAL	133		-42.461		1.00 23.30	A	C
00	ATOM	253	0	VAL	133		-43.110		1.00 21.98	A	0
30	MOTA	254	N	GLN	134		-41.214		1.00 25.25	A	N
	MOTA	255	CA	GLN	134		-40.505		1.00 28.42	A	C
	MOTA	256	CB	GLN	134		-39.001		1.00 31.35	Α	C
	MOTA	257	CG	GLN	134		-38.496		1.00 35.93	A	C
0.5	MOTA	258	CD	GLN	134		-37.018		1.00 38.86	A	C
35	MOTA	259		GLN	134		-36.224		1.00 40.75	A	0
	MOTA	260		GLN	134		-36.634		1.00 40.53	Α	N
	MOTA	261	С	GLN	134		-40.739		1.00 28.55	Α	C
	MOTA	262	0	GLN	134		-40.113		1.00 28.59	A	0
40	MOTA	263	N	PHE	135	-11.933			1.00 27.76	A	N
40	ATOM	264	CA	PHE	135		-41.834		1.00 27.25	A	С
	ATOM	265	CB	PHE	135		-41.361		1.00 27.33	A	C
	ATOM	266	CG	PHE	135	-9.653					
	ATOM	267		PHE	135		-38.978		1.00 27.07	A	C
45	MOTA	268		PHE	135		-39.363		1.00 27.37	A	C
45	MOTA	269		PHE	135		-37.595		1.00 26.82	A	C
	ATOM	270	CE2		135		-37.979		1.00 27.26	A	C
	ATOM	271	CZ	PHE	135		-37.096		1.00 26.50	A	C
	MOTA	272	C	PHE	135		-43.256		1.00 26.66	A	C
50	ATOM	273	0	PHE	135		-43.843		1.00 26.40	A	0
30	ATOM	274	N	ARG	136		-43.784		1.00 26.15	Α	
	MOTA	275	CA	ARG	136		-45.129		1.00 25.96	A	C
	ATOM	276	CB	ARG	136		-45.115		1.00 26.56	A	C
	MOTA	277	CG	ARG	136		44.063		1.00 29.01	A	C
55	ATOM	278	CD	ARG	136		43.086		1.00 31.35	A	
	ATOM	279	NE C7	ARG	136		40.621		1.00 34.32	A	
	MOTA MOTA	280 281	CZ	ARG	136		40.621		1.00 35.38	A	
	ATOM	281		L ARG	136		40.660		1.00 34.41	A	
	AIOM	202	NH	2 ARG	136	-9.442	-39.452	91.073	1.00 37.45	A	N

-174-

	ATOM	283	С	ARG	136	-10.530	-46.179	94.623	1.00 25.24	A	C
	ATOM	284	0	ARG	136	-9.486	-46.819	94.496	1.00 24.38	A	ŏ
	ATOM	285	N	PRO	137		-46.371	95.662	1.00 24.16		
	ATOM	286	CD	PRO	137		-45.707	95.999		A	N
5	MOTA	287	CA	PRO	137		-47.366		1.00 23.61	A	C
_	ATOM	288	CB	PRO	137			96.672	1.00 23.41	A	C
	ATOM						-47.081	97.790	1.00 23.30	A	C
		289	CG	PRO	137		-46.654	97.013	1.00 23.80	A	C
	ATOM	290	C	PRO	137		-48.776	96.149	1.00 23.31	A	C
40	ATOM	291	0	PRO	137		-49.115	95.545	1.00 22.63	Α	0
10	MOTA	292	N	PRO	138	-10.147	-49.620	96.358	1.00 23.12	A	N
	ATOM	293	CD	PRO	138	-8.801	-49.369	96.907	1.00 23.19	A	C
	ATOM	294	CA	PRO	138		-50.993	95.875	1.00 23.26	A	C
	ATOM	295	СВ	PRO	138		-51.679	96.450	1.00 23.20		
	MOTA	296	CG	PRO	138		-50.578			A	C
15	ATOM	297	C	PRO	138			96.421	1.00 24.11	A	C
	ATOM	298	Ö				-51.547	96.464	1.00 22.75	A	C
				PRO	138		-51.142	97.556	1.00 22.46	Α	0
	MOTA	299	N	ALA	139		-52.468	95.748	1.00 21.31	Α	N
	MOTA	300	CA	ALA	139		-53.061	96.193	1.00 21.53	A	C
00	MOTA	301	CB	ALA	139		-54.024	95.114	1.00 21.98	Α	C
20	MOTA	302	С	ALA	139	-13.442	-53.774	97.556	1.00 21.59	A	C
	ATOM	303	0	ALA	139	-14.439	-53.750	98.282	1.00 20.89	A	ō
	ATOM	304	N	HIS	140		-54.405	97.916	1.00 21.14	A	N
	ATOM	305	CA	HIS	140		-55.107	99.199	1.00 21.14		
	ATOM	306	CB	HIS	140		-55.903	99.342		A	C
25	ATOM	307	CG	HIS	140		-55.062		1.00 22.63	A	C
	ATOM	308		HIS				99.725	1.00 21.19	A	C
	ATOM				140			100.936	1.00 21.22	A	C
		309		HIS	140		-54.347	98.804	1.00 20.38	A	N
	MOTA	310		HIS	140		-53.650	99.431	1.00 21.24	A	C
20	ATOM	311		HIS	140			100.726	1.00 22.01	A	N
30	MOTA	312	С	HIS	140		-54.153		1.00 22.47	A	C
	MOTA	313	0	HIS	140	-12.605	-54.586	101.518	1.00 22.16	A	0
	ATOM	314	N	LEU	141	-12.251	-52.857	100.134	1.00 23.58	A	N
	ATOM	315	CA	LEU	141	-12.364	-51.827	101.166	1.00 23.85	A	C
	ATOM	316	CB	LEU	141	-11.777	-50.520	100.634	1.00 23.18	A	C
35	ATOM	317	CG	LEU	141	-10.527	-49 937	101.294	1.00 23.18		
	ATOM	318		LEU	141	-9 667	-51 037	101.903		A	C
	ATOM	319		LEU	141			101.903	1.00 22.26	A	С
	ATOM	320	C	LEU	141				1.00 21.25	A	C
	ATOM	321					-51.599		1.00 24.27	A	C
40			0	LEU	141	-14.066	-51.148	102.718	1.00 23.20	Α	0
70	ATOM	322	N	PHE	142	-14.759	-51.902	100.719	1.00 24.16	Α	N
	MOTA	323	CA	PHE	142	-16.173	-51.717	101.032	1.00 25.36	A	С
	MOTA	324	CB	PHE	142	-17.017	-51.773	99.752	1.00 23.10	A	С
	ATOM	325	CG	PHE	142	-16.898	-50.549	98.901	1.00 22.13	Α	C
	MOTA	326	CD1	PHE	142	-17.570	-49.385	99.240	1.00 22.32	A	Ċ
45	ATOM	327	CD2	PHE	142	-16.087		97.780	1.00 22.24	A	Č
	ATOM	328		PHE	142	-17.432		98.467	1.00 22.25	A	C
	ATOM	329		PHE	142	-15.944		97.006	1.00 22.23		
	ATOM	330	CZ	PHE	142		-48.242	97.349		A	C
	ATOM	331	C	PHE	142		-52.771		1.00 20.96	A	C
50	ATOM	332							1.00 26.65	A	С
00			0	PHE	142		-53.914		1.00 26.20	Α	0
	ATOM	333	N	ILE	143		-52.380		1.00 28.79	Α	N
	MOTA	334	CA	ILE	143		~53.310		1.00 31.69	Α	С
	MOTA	335	CB	ILE	143		-52.630		1.00 32.78	A	C
	MOTA	336	CG2		143	-18.682	-51.372	105.382	1.00 33.71	A	Ċ
55	MOTA	337	CG1	ILE	143		-52.300		1.00 33.80	A	C
	ATOM	338	CD1	ILE	143		-51.225		1.00 35.73	A	C
	ATOM	339	С	ILE	143		-54.449		1.00 32.40	A	C
	ATOM	340	0	ILE	143		-54.277		1.00 32.40	A	
	- 1		-				J=.411	101.070	1.00 31.9/	A	0

-175-

	MOTA	341	N	HIS	144	-18.967			1.00 33.54	A	N
	MOTA	342	CA	HIS	144	-19.568	-56.769	103.023	1.00 35.74	A	С
	MOTA	343	CB	HIS	144	-20.924			1.00 36.54	Α	C
_	MOTA	344	CG	HIS	144	-21.853			1.00 37.08	A	C
5	MOTA	345	CD2		144	-22.508			1.00 36.90	A	C
	MOTA	346	ND1	HIS	144	-22.207			1.00 37.27	A	N
	MOTA	347	CE1	HIS	144	-23.037	-55.349	105.156	1.00 37.23	A	C
	MOTA	348	NE2	HIS	144	-23.235	-54.321	104.350	1.00 37.35	A	N
	MOTA	349	C	HIS	144		-57.317		1.00 36.21	A	C
10	MOTA	350	0	HIS	144		-57.751		1.00 36.04	Α	0
	MOTA	351	N	HIS	145		-57.289		1.00 37.47	Α	N
	MOTA	352	CA	HIS	145			101.236	1.00 38.79	A	C
	MOTA	353	CB	HIS	145			100.471	1.00 38.32	A	C
	MOTA	354	CG	HIS	145	-16.612		99.379	1.00 38.92	A	C
15	MOTA	355	CD2	HIS	145	-17.687	-55.260	99.416	1.00 38.33	A	С
	ATOM	356	ND1	HIS	145	-16.436	-56.427	98.056	1.00 38.61	A	N
	ATOM	357	CE1	HIS	145	-17.365	-55.840	97.325	1.00 38.59	A	C
	ATOM	358		HIS	145	-18.138	-55.127	98.125	1.00 39.24	A	N
	MOTA	359	С	HIS	145	-15.248	-58.564	101.914	1.00 39.68	Α	C
20	ATOM	360	0	HIS	145	-14.995	-58.406	103.110	1.00 40.45	Α	0
	ATOM	361	N	GLN	146	-14.593	-59.417	101.134	1.00 40.62	A	N
	ATOM	362	CA	GLN	146	-13.495	-60.232	101.632	1.00 40.83	Α	С
	ATOM	363	CB	GLN	146			100.899	1.00 42.96	A	C
	MOTA	364	CG	GLN	146	-13.528	-61.487	99.376	1.00 46.15	A	С
25	MOTA	365	CD	GLN	146	-13.498	-62.850	98.685	1.00 48.68	A	С
	MOTA	366	OE1	GLN	146	-14.422	-63.659	98.824	1.00 49.88	Α	0
	ATOM	367	NE2	GLN	146	-12.430	-63.105	97.934	1.00 49.37	A	N
	MOTA	368	С	GLN	146	-12.193	-59.464	101.412	1.00 39.30	A	C
	MOTA	369	0	GLN	146	-12.075	-58.685	100.467	1.00 39.67	A	0
30	MOTA	370	N	PRO	147	-11.201	-59.664	102.292	1.00 37.59	Α	N
	MOTA	371	CD	PRO	147	-11.172	-60.620	103.411	1.00 37.45	A	C
	MOTA	372	CA	PRO	147	-9.917	-58.969	102.165	1.00 35.57	A	C
	MOTA	373	CB	PRO	147			103.367	1.00 36.50	A	C
	MOTA	374	CG	PRO	147	-9.700	-60.851	103.580	1.00 37.77	Α	С
35	ATOM	375	C	PRO	147			100.835	1.00 33.38	Α	C
	MOTA	376	0	PRO	147	-9.528		100.094	1.00 33.33	Α	0
	ATOM	377	N	LEU	148	-8.227			1.00 30.98	Α	N
	MOTA	378	CA	LEU	148		-58.458		1.00 29.30	Α	С
	MOTA	379	CB	LEU	148		-57.469		1.00 29.16	A	С
40	MOTA	380	CG	LEU	148		-56.372		1.00 29.82	A	С
	MOTA	381		LEU	148		-55.910		1.00 29.71	A	С
	MOTA	382	CD2	LEU	148		-56.870		1.00 29.27	A	С
	MOTA	383	С	LEU	148		-59.865		1.00 27.66	A	С
	ATOM	384	0	LEU	148			100.085	1.00 26.44	Α	0
45	MOTA	385	N	PRO	149		-60.483		1.00 26.63	A	N
	MOTA	386	CD	PRO	149		-60.093		1.00 26.30	Α	С
	MOTA	387	CA	PRO	149		-61.82		1.00 26.49	A	
	MOTA	388	CB	PRO	149		-62.192		1.00 26.48		
	MOTA	389		PRO	149		-61.43				
50	MOTA	390		PRO	149	-4.993					
	ATOM	391		PRO	149	-4.372					
	ATOM	392		THR	150	-4.402					
	MOTA	393		THR	150		-63.13				
	MOTA	394		THR	150		-64.63				
55	MOTA	395			150		L -65.03				
	MOTA	396			150		2 -64.88				
	MOTA	397		THR	150		3 -62.61				
	ATOM	398	0	THR	150	-1.15	5 -61.93	3 97.123	1.00 25.67	A	0

-176-

	MOTA	399	N	LEU	151	-2.652	-62.924	95.766	1.00 26.09	A	N
	MOTA	400	CA	LEU	151		-62.520	94.543	1.00 27.02	A	C
	MOTA	401	CB	LEU	151		-63.692	93.548	1.00 28.10	A	C
_	MOTA	402	CG	LEU	151		-64.622	93.469	1.00 28.68	A	C
5	MOTA	403	CD1		151		-64.874	94.830	1.00 28.89	A	C
	ATOM	404	CD2		151		-65.927	92.809	1.00 28.50	A	C
	MOTA	405	C	LEU	151		-61.258	93.865	1.00 26.77	A	C
	MOTA	406	0	LEU	151		-60.827	92.849	1.00 26.56	A	0
40	ATOM	407	N	ALA	152		-60.659	94.422	1.00 26.15	A	N
10	MOTA	408	CA	ALA	152		-59.442	93.836	1.00 25.48	A	C
	MOTA	409	CB	ALA	152		-59.064	94.544	1.00 25.10	A	C
	ATOM	410	C	ALA	152		-58.290	93.937	1.00 24.90	A	C
	ATOM	411	0	ALA	152		-58.073	94.985	1.00 23.72	A	0
15	ATOM	412	N	PRO	153		-57.544	92.841	1.00 24.54	A	N
15	ATOM	413	CD	PRO	153		-57.751	91.463	1.00 25.59	A	C
	ATOM	414	CA	PRO	153		-56.435	92.919	1.00 24.98	A	C
	ATOM	415	CB	PRO	153		-55.859	91.495	1.00 25.27	A	C
	ATOM	416	CG	PRO	153		-56.374 -55.421	90.870	1.00 25.95	A	C
20	MOTA MOTA	417 418	C O	PRO PRO	153 153		-55.182	93.993 94.220	1.00 25.30 1.00 25.69	A	C
20	MOTA	419	N	VAL	154		-54.845	94.220	1.00 25.69	A A	N
	MOTA	420	CA	VAL	154		-53.884	95.730	1.00 24.93	A	C
	ATOM	421	CB	VAL	154		-54.044	96.884	1.00 25.03	A	C
	ATOM	422		VAL	154		-53.454	96.484	1.00 26.07	A	c
25	ATOM	423		VAL	154		-53.391	98.148	1.00 27.60	A	Ċ
	ATOM	424	C	VAL	154		-52.432	95.245	1.00 25.24	A	č
	ATOM	425	ŏ	VAL	154		-51.531	95.980	1.00 25.07	A	ō
	ATOM	426	N	LEU	155		-52.214	94.010	1.00 24.31	A	N
	ATOM	427	CA	LEU	155	-1.150	-50.875	93.418	1.00 24.23	A	C
30	ATOM	428	СВ	LEU	155		-50.977	91.910	1.00 24.21	A	С
	ATOM	429	CG	LEU	155	-0.776	-49.663	91.118	1.00 25.59	A	C
	ATOM	430	CD1	LEU	155	0.261	-48.739	91.744	1.00 24.34	Α	C
	MOTA	431	CD2	LEU	155	-0.426	-49.962	89.658	1.00 24.80	A	C
	MOTA	432	Ç	LEU	155	-2.418	-50.038	93.661	1.00 23.18	A	C
35	MOTA	433	0	LEU	155		-48.915	94.149	1.00 23.96	Α	0
	MOTA	434	N	PRO	156		-50.569	93.331	1.00 22.69	A	N
	MOTA	435	CD	PRO	156		-51.848	92.684	1.00 22.19	A	С
	MOTA	436	CA	PRO	156		-49.757	93.571	1.00 22.08	A	C
40	MOTA	437	CB	PRO	156		-50.698	93.171	1.00 22.24	A	C
40	MOTA	438	CG	PRO	156		-51.539	92.086	1.00 22.14	A	C
	ATOM	439	C	PRO	156		-49.277	95.031	1.00 22.20	A	C
	ATOM	440	0	PRO	156		-48.122	95.287 95.980	1.00 20.87	A	
	ATOM	441	N	LEU	157 157		-50.164 -49.813	97.397	1.00 20.93 1.00 20.80	A	N
45	ATOM ATOM	442 443	CA CB	LEU	157		-51.046	98.269	1.00 20.80	A A	C
73	ATOM	444	CG	LEU LEU	157		-50.793	99.783	1.00 19.44	A	C
	ATOM	445		LEU	157		-50.152	100.220	1.00 19.55	A	C
	ATOM	446		LEU	157		-52.113	100.522	1.00 16.20	A	C
	ATOM	447	C	LEU	157		-48.738	97.715	1.00 20.74	A	Č
50	ATOM	448	ŏ	LEU	157		-47.774	98.422	1.00 20.79	A	ŏ
•	ATOM	449	N	VAL	158		-48.911	97.186	1.00 20.78	A	N
	ATOM	450	CA	VAL	158		-47.962	97.387	1.00 20.77	Α	C
	ATOM	451	СВ	VAL	158		-48.480	96.704		A	Č
	ATOM	452		L VAL	158		-47.402	96.720		A	
55	ATOM	453		VAL	158		-49.743	97.420		A	
	ATOM	454		VAL	158		-46.583	96.810		A	
	ATOM	455		VAL	158		-45.549			A	
	ATOM	456		THR	159	-2.293	-46.575	95.621	1.00 21.17	A	

-177-

	MOTA	457	CA	THR	159		-45.334	94.956	1.00 21.04	A	C
	MOTA	458	CB	THR	159	_	-45.606	93.484	1.00 21.88	A	C
	MOTA	459		THR	159		-46.413	92.882	1.00 22.76	A	0
E	MOTA	460		THR	159		-44.308	92.710	1.00 21.05	A	C
5	ATOM	461	С	THR	159		-44.677	95.682	1.00 20.47	A	C
	MOTA	462	0	THR	159		-43.449	95.721	1.00 20.97	A	0
	ATOM	463	N	HIS	160		-45.500	96.252	1.00 19.61	A	N
	MOTA	464	CA	HIS	160		-45.009	97.008	1.00 20.01	A	C
10	MOTA	465	CB	HIS	160		-46.161	97.423	1.00 20.08	A	C
10	MOTA	466	CG	HIS	160		-45.744	98.354	1.00 20.94	A	C
	MOTA	467	CD2		160		-45.999	99.669	1.00 20.95	A	C
	MOTA	468	ND1		160		-44.925	97.965	1.00 21.19	A	N
	MOTA	469	CE1		160		-44.691	99.000	1.00 20.93	A	C
1=	MOTA	470		HIS	160	-	-45.331		1.00 20.20	A	N
15	MOTA	471	С	HIS	160		-44.308	98.254	1.00 19.95	A	С
	MOTA	472	0	HIS	160		-43.219	98.600	1.00 20.42	A	0
	MOTA	473	N	PHE	161		-44.933	98.920	1.00 18.59	A	N
	MOTA	474	CA	PHE	161		-44.345		1.00 18.56	A	C
20	MOTA	475	CB	PHE	161		-45.327	100.735	1.00 18.23	A	C
20	MOTA	476	CG	PHE	161		-46.356		1.00 17.32	A	C
	MOTA	477		PHE	161		-46.314		1.00 16.89	A	C
	MOTA	478		PHE	161		-47.362		1.00 18.24	A	C
	MOTA	479		PHE	161		-47.255		1.00 17.84	A	C
25	MOTA	480		PHE	161		-48.308		1.00 17.78	A	C
23	ATOM	481	CZ	PHE	161		-48.253		1.00 16.70	A	C
	MOTA	482	C	PHE	161		-43.030		1.00 19.43	A	C
	MOTA	483	0	PHE	161		-42.041		1.00 18.14	A	0
	MOTA	484	N	ALA	162		-43.019		1.00 19.79	A	N
30	MOTA	485	CA	ALA	162		-41.809		1.00 21.41	A	C
30	MOTA	486	CB	ALA	162		-42.061		1.00 20.88	A	C
	ATOM	487	C	ALA	162		-40.674		1.00 22.02	A	C
	MOTA	488	0	ALA	162		-39.545		1.00 22.29	A A	N O
	MOTA	489	N	ASP	163		-40.991		1.00 22.30		C
35	MOTA	490	CA	ASP	163		40.012		1.00 22.87 1.00 23.81	A	
95	ATOM	491	CB	ASP	163		-40.626			A	C
	ATOM	492	CG	ASP	163)40.804 5 -41.605		1.00 25.70 1.00 24.91	A A	0
	ATOM	493		ASP	163		-41.605 -40.134		1.00 25.54	A	0
	ATOM	494	OD2		163		-39.468		1.00 23.34	A	c
40	ATOM	495	C	ASP	163		-39.400 5 -38.254		1.00 23.27	A	0
.0	MOTA	496	0	ASP ILE	163 164		5 -40.346		1.00 22.58	A	N
	ATOM ATOM	497 498	N CA	ILE	164			100.527	1.00 22.00		C
		499	CB	ILE	164			101.261	1.00 21.65	A	C
	ATOM ATOM	500		2 ILE	164			100.302	1.00 19.34	A	Č
45	ATOM	501		LILE	164			101.807	1.00 20.52		Č
. •	ATOM	502		LILE	164			102.530	1.00 18.21		č
	ATOM	502		ILE	164			7 101.490			
	ATOM	504		ILE	164			102.281			
	ATOM	505		ASN	165			101.425			
50	MOTA	506		ASN	165			3 102.289			
- •	MOTA	507		ASN	165			9 102.200			
	MOTA	508			165			7 102.962			
	MOTA	509		ASN 1 ASN	165			3 103.784			
	MOTA	510		2 ASN	165			0 102.703			
55	MOTA	511		ASN	165			4 101.858			
•	ATOM	512		ASN	165			B 102.690			
	ATOM	513		THR	166			7 100.549			
	ATOM	514			166		8 -35.99				
	111 OF	217			200						_

-178-

	ATOM	515	СВ	THR	166		-36.082	98.448	1.00 25.05	A	C
	MOTA	516		THR	166		-36.830	98.166	1.00 25.95	A	0
	MOTA	517	CG2	THR	166		-34.689	97.834	1.00 24.40	A	С
_	MOTA	518	C	THR	166		-35.168		1.00 24.71	A	C
5	MOTA	519	0	THR	166		-34.020		1.00 25.33	A	0
	ATOM	520	N	PHE	167		-35.765		1.00 23.87	A	N
	MOTA	521	CA	PHE	167		-35.125		1.00 23.69	A	C
	MOTA	522	CB	PHE	167		-36.132		1.00 23.28	A	C
	ATOM	523	CG	PHE	167			100.719	1.00 23.25	Α	C
10	ATOM	524		PHE	167			100.184	1.00 23.28	A	C
	MOTA	525	CD2	PHE	167			101.842	1.00 22.82	A	C
	ATOM	526		PHE	167			100.757	1.00 21.97	A	С
	MOTA	527	CE2	PHE	167			102.427	1.00 22.68	A	C
	MOTA	528	CZ	PHE	167			101.880	1.00 22.73	A	С
15	MOTA	529	С	PHE	167	-6.440	-34.611	101.755	1.00 24.07	A	C
	MOTA	530	0	PHE	167	-6.676	-33.427	101.996	1.00 24.74	Α	0
	MOTA	531	N	MET	168	-6.161	-35.508	102.702	1.00 22.88	A	N
	ATOM	532	CA	MET	168	-6.133	-35.168	104.123	1.00 22.54	Α	C
	MOTA	533	CB	MET	168	-5.844	-36.420	104.974	1.00 20.50	A	C
20	MOTA	534	CG	MET	168	-7.020	-37.378	105.090	1.00 19.43	A	C
	ATOM	535	SD	MET	168	-6.792	-38.627	106.404	1.00 16.80	A	S
	MOTA	536	CE	MET	168	-5.899	-39.880	105.499	1.00 19.32	Α	С
	ATOM	537	С	MET	168	-5.137	-34.065	104.472	1.00 22.25	A	C
	ATOM	538	0	MET	168	-5.459	-33.160	105.226	1.00 21.58	A	0
25	MOTA	539	N	VAL	169	-3.928	-34.144	103.932	1.00 22.92	A	N
	MOTA	540	CA	VAL	169	-2.927	-33.112	104.186	1.00 23.69	A	C
	MOTA	541	CB	VAL	169	-1.635	-33.375	103.383	1.00 24.08	A	C
	ATOM	542	CG1	VAL	169	-0.668	-32.208	103.555	1.00 25.04	Α	С
	ATOM	543	CG2	VAL	169	-0.981	-34.661	103.863	1.00 24.66	Α	C
30	ATOM	544	С	VAL	169	-3.470	-31.733	103.794	1.00 24.06	Α	С
	ATOM	545	0	VAL	169	-3.335	-30.759	104.546	1.00 23.08	A	0
	ATOM	546	N	LEU	170	-4.084	-31.656	102.616	1.00 24.09	A	N
	ATOM	547	CA	LEU	170	-4.650	-30.404	102.131	1.00 24.47	A	C
	ATOM	548	CB	LEU	170	-5.170	-30.587	100.702	1.00 25.76	Α	С
35	MOTA	549	CG	LEU	170	-4.109	-30.969	99.660	1.00 27.02	A	С
	ATOM	550	CD1	LEU	170	-4.776	-31.173	98.303	1.00 27.49	Α	С
	ATOM	551	CD2	LEU	170	-3.037	-29.881	99.575	1.00 27.84	Α	С
	ATOM	552	С	LEU	170	-5.772	-29.919	103.054	1.00 24.53	Α	С
	ATOM	553	0	LEU	170	-5.954	-28.715	103.246	1.00 24.40	Α	0
40	ATOM	554	N	GLN	171	-6.519	-30.855	103.637	1.00 23.66	A	N
	ATOM	555	CA	GLN	171	-7.589	-30.484	104.550	1.00 23.20	A	C
	ATOM	556	СВ	GLN	171	-8.482	-31.692	104.856	1.00 22.89	A	C
	ATOM	557	CG	GLN	171	-9.301	-32.169	103.657	1.00 22.15	Α	C
	ATOM	558	CD	GLN	171	-10.227	-31.085	103.108	1.00 21.39	A	С
45	ATOM	559	OE1	GLN	171	-11.164	-30.644	1 103.777	1.00 20.79	Α	0
	MOTA	560	NE	2 GLN	171	-9.960	-30.650	101.888	1.00 20.38	Α	N
	ATOM	561	С	GLN	171	-7.004	-29.920	105.841	1.00 23.71	Α	С
	ATOM	562	0	GLN	171	-7.621	29.073	L 106.485	1.00 22.77	A	0
	ATOM	563		VAL	172	-5.820	-30.390	106.232	1.00 24.17	Α	N
50	ATOM	564		VAL	172	-5.195	-29.868	3 107.445	1.00 25.12	Α	
	MOTA	565		VAL	172	-3.989	-30.71	1 107.893	1.00 25.29	A	
	MOTA	566		l VAL	172			5 109.034	1.00 23.34	A	
	MOTA	567		2 VAL	172			8 108.339	1.00 24.47	Α	
	MOTA	568		VAL	172			0 107.193	1.00 25.52	A	
55	ATOM	569		VAL	172			5 108.057		Α	
_	ATOM	570		ILE	173			5 106.010			
	ATOM	571			173			5 105.646			
	ATOM	572		ILE	173			2 104.231			
		_									

-179-

	MOTA	573	CG2		173		-25.491		1.00 26.79	A	C
	MOTA	574		ILE	173		-27.822		1.00 27.16	A	C
	MOTA	575		ILE	173		-27.937		1.00 27.08	A	С
_	MOTA	576	С	ILE	173		-25.919		1.00 27.47	A	С
5	MOTA	577	0	ILE	173			106.320	1.00 27.14	A	0
	MOTA	578		LYS	174			105.122	1.00 27.73	A	N
	MOTA	579	CA	LYS	174			105.141	1.00 28.31	A	C
	ATOM	580	CB	LYS	174			104.296	1.00 28.44	A	С
	ATOM	581	CG	LYS	174			102.803	1.00 29.80	A	C
10	ATOM	582	CD	LYS	174			101.975	1.00 31.27	A	C
	ATOM	583	CE	LYS	174			101.958	1.00 32.16	Α	C
	MOTA	584	NZ	LYS	174			101.116	1.00 34.46	A	N
	MOTA	585	С	LYS	174			106.570	1.00 28.11	A	С
	MOTA	586	0	LYS	174	-	-24.147		1.00 28.60	A	0
15	MOTA	587	N	PHE	175			107.429	1.00 27.63	A	N
	MOTA	588	CA	PHE	175			108.834	1.00 27.68	A	C
	MOTA	589	CB	PHE	175			109.524	1.00 27.35	A	C
	MOTA	590	CG	PHE	175			111.029	1.00 27.54	Α	C
	MOTA	591	CD1	PHE	175			111.651	1.00 27.14	A	C
20	MOTA	592		PHE	175			111.822	1.00 27.58	A	C
	MOTA	593	CE1	PHE	175	-9.129	-27.040	113.039	1.00 26.74	A	С
	MOTA	594	CE2	PHE	175			113.215	1.00 27.74	A	C
	ATOM	595	CZ	PHE	175	-8.010	-27.296	113.823	1.00 27.47	A	С
	MOTA	596	С	PHE	175	-7.042	-25.094	109.551	1.00 28.52	Α	C
25	MOTA	597	0	PHE	175	-7.558	-24.244	110.268	1.00 27.62	A	0
	MOTA	598	N	THR	176	-5.731	-25.148	109.343	1.00 29.79	A	N
	MOTA	599	CA	THR	176	-4.824	-24.204	109.985	1.00 31.23	A	C
	MOTA	600	CB	THR	176			109.789	1.00 30.67	Α	C
	MOTA	601	OG1	THR	176	-3.022	-24.563	108.399	1.00 30.30	A	0
30	MOTA	602	CG2	THR	176	-3.138	-26.036	110.306	1.00 31.22	A	C
	MOTA	603	C	THR	176			109.479	1.00 32.33	A	C
	MOTA	604	0	THR	176			110.232	1.00 32.61	A	0
	MOTA	605	N	LYS	177	-5.358	-22.633	108.207	1.00 33.30	A	N
	MOTA	606	CA	LYS	177	-5.565	-21.319	107.602	1.00 34.34	A	C
35	MOTA	607	CB	LYS	177			106.105	1.00 35.54	A	С
	MOTA	608	CG	LYS	177			105.310	1.00 38.15	Α	C
	ATOM	609	CD	LYS	177			105.087	1.00 39.75	A	С
	MOTA	610	CE	LYS	177			104.434	1.00 40.78	Α	C
	MOTA	611	NZ	LYS	177			103.187	1.00 41.40	A	N
40	MOTA	612	С	LYS	177			108.243	1.00 34.59	Α	С
	MOTA	613	0	LYS	177			108.153	1.00 35.04	A	0
	MOTA	614	N	ASP	178			108.874		A	
	MOTA	615	CA	ASP	178			109.543	1.00 34.02	Α	С
	MOTA	616	CB	ASP	178			109.445	1.00 34.24	A	С
45	MOTA	617	CG	ASP	178			108.129	1.00 34.92	A	C
	ATOM	618		ASP	178			107.277	1.00 35.28	A	0
	MOTA	619	OD2	ASP	178			2 107.950	1.00 36.67	A	0
	MOTA	620	C	ASP	178			9 111.013	1.00 33.84	Α	С
	MOTA	621	0	ASP	178			5 111.752	1.00 34.10	A	0
50	MOTA	622		LEU	179			2 111.439	1.00 33.64	Α	Ŋ
	MOTA	623		LEU	179			2 112.819	1.00 33.48	Α	С
	MOTA	624		LEU	179			113.398	1.00 32.20	Α	С
	MOTA	625		LEU	179			7 113.240	1.00 31.98	Α	С
	ATOM	626		LEU	179			1 113.963	1.00 31.56	Α	_
55	ATOM	627			179			5 113.793	1.00 30.73	A	_
	MOTA	628	С	LEU	179			1 112.834		Α	
	MOTA	629	0	LEU	179			2 112.464		A	-
	MOTA	630	N	PRO	180	-6.703	-17.86	3 113.252	1.00 34.34	Α	N

-180-

	ATOM	631	CD	PRO	180	-8.097 -17.743 113.718 1.00 34.10	A	C
	ATOM	632	CA	PRO	180	-6.028 -16.564 113.312 1.00 34.65	A	C
	MOTA	633	CB	PRO	180	-6.994 -15.725 114.135 1.00 34.81	A	C
_	MOTA	634	CG	PRO	180	-8.322 -16.250 113.675 1.00 34.48	A	C
5	ATOM	635	С	PRO	180	-4.631 -16.606 113.916 1.00 35.01	A	C
	ATOM	636	0	PRO	180	-3.680 -16.112 113.320 1.00 34.47	A	0
	MOTA	637	N	VAL	181	-4.501 -17.208 115.092 1.00 35.81	A	N
	ATOM	638	CA	VAL	181	-3.200 -17.275 115.745 1.00 36.75	A	C
	ATOM	639	CB	VAL	181	-3.311 -17.889 117.149 1.00 37.21	A	C
10	ATOM	640	CG1	VAL	181	-1.931 -18.014 117.762 1.00 38.68	A	C
	ATOM	641	CG2	VAL	181	-4.189 -17.007 118.032 1.00 38.14	Α	C
	ATOM	642	С	VAL	181	-2.165 -18.051 114.935 1.00 36.94	A	C
	MOTA	643	0	VAL	181	-0.978 -17.730 114.976 1.00 36.68	A	Ō
	ATOM	644	N	PHE	182	-2.604 -19.069 114.198 1.00 37.05	Α	N
15	ATOM	645	CA	PHE	182	-1.677 -19.847 113.378 1.00 37.75	A	c
	ATOM	646	СВ	PHE	182	-2.325 -21.141 112.878 1.00 37.39	A	C
	ATOM	647	CG	PHE	182	-1.431 -21.945 111.972 1.00 37.39		c
	ATOM	648		PHE	182	-0.475 -22.806 112.500 1.00 37.05	A	Č
	ATOM	649			182	-1.513 -21.805 110.590 1.00 37.03	A	C
20	ATOM	650		PHE	182	0.387 -23.517 111.663 1.00 36.56	A	C
	ATOM	651	CE2		182	-0.653 -22.511 109.746 1.00 37.00		C
	ATOM	652	CZ	PHE	182	0.297 -23.368 110.286 1.00 36.96	A	
	ATOM	653	C	PHE	182		A	C
	MOTA	654	Ö	PHE	182	-1.242 -19.036 112.163	A	C
25	ATOM	655	N	ARG	183		A	0
2.0	ATOM	656	CA	ARG	183	-2.214 -18.426 111.499 1.00 39.10	A	N
	ATOM	657	CB	ARG	183	-1.948 -17.630 110.314 1.00 40.37 -3.268 -17.242 109.661 1.00 40.60	A	C
	ATOM	658	CG	ARG	183		A	C
	ATOM	659	CD	ARG	183		A	C
30	ATOM	660	NE	ARG	183		A	C
00	ATOM	661	CZ	ARG	183		A	N
	MOTA	662	NH1		183	-5.001 -16.419 105.160 1.00 39.62 -6.132 -17.079 105.370 1.00 39.80	A	C
	ATOM	663	NH2		183		A	N
	ATOM	664		ARG	183		A	N
35	MOTA	665	C		183		A	C
33			0	ARG		-0.433 -15.856 109.747 1.00 41.39	A	0
	ATOM	666	N	SER	184	-1.215 -15.910 111.858 1.00 42.46	A	N
	MOTA	667	CA	SER	184	-0.484 -14.728 112.292 1.00 43.82	A	C
	MOTA	668	CB	SER	184	-1.051 -14.236 113.620 1.00 44.39	Α	С
40	MOTA	669	OG	SER	184	-0.499 -12.984 113.959 1.00 47.04	A	0
40	ATOM	670	C	SER	184	1.016 -14.996 112.439 1.00 44.32	A	C
	ATOM	671	0	SER	184	1.813 -14.060 112.538 1.00 44.62	A	
	ATOM	672	N	LEU	185	1.395 -16.273 112.459 1.00 44.27		
	MOTA	673	CA	LEU	185	2.796 -16.666 112.578 1.00 44.64	A	
AE	MOTA	674	CB	LEU	185	2.903 -18.150 112.945 1.00 43.86	A	
45	MOTA	675	CG	LEU	185	2.344 -18.644 114.282 1.00 44.09	A	
	MOTA	676		LEU	185	2.459 -20.166 114.362 1.00 42.72	A	
	MOTA	677		LEU	185	3.103 -17.992 115.423 1.00 43.21	A	
	ATOM	678	C	LEU	185	3.510 -16.447 111.248 1.00 45.42		
50	MOTA	679	0	LEU	185	2.876 -16.405 110.194 1.00 45.54		
50	ATOM	680	N	PRO	186	4.844 -16.304 111.278 1.00 46.26		
	MOTA	681	CD	PRO	186	5.775 -16.356 112.418 1.00 46.30		
	MOTA	682	CA	PRO	186	5.566 -16.103 110.018 1.00 46.87		
	MOTA	683	CB	PRO	186	7.008 -15.893 110.477 1.00 46.47		
	MOTA	684	CG	PRO	186	7.084 -16.693 111.741 1.00 47.00		
55	ATOM	685	C	PRO	186	5.390 -17.348 109.144 1.00 47.62		
	MOTA	686	0	PRO	186	5.308 -18.463 109.659 1.00 48.13		
	MOTA	687	N	ILE	187	5.328 -17.154 107.830 1.00 47.94		
	MOTA	688	CA	ILE	187	5.131 -18.256 106.891 1.00 47.82	Α	С

-181-

	ATOM	689	СВ	ILE	187	5.236	-17.749	105.423	1.00 48.13	A	C
	ATOM	690	CG2	ILE	187	6.601	-17.105	105.182	1.00 48.93	A	C
	ATOM	691	CG1	ILE	187	4.975	-18.895	104.442	1.00 48.18	A	С
_	MOTA	692	CD1	ILE	187	6.169	-19.808	104.180	1.00 48.34	A	C
5	MOTA	693	С	ILE	187	6.055	-19.460	107.095	1.00 47.81	A	C
	MOTA	694	0	ILE	187	5.614	-20.602	106.967	1.00 47.87	A	0
	ATOM	695	N	GLU	188	7.327	-19.221	107.405	1.00 47.20	A	N
	ATOM	696	CA	GLU	188	8.265	-20.320	107.619	1.00 46.46	Α	С
	ATOM	697	CB	GLU	188	9.702	-19.800	107.799	1.00 47.64	A	C
10	ATOM	698	CG	GLU	188	9.846	-18.469	108.533	1.00 50.01	A	C
	ATOM	699	CD	GLU	188	9.421	-17.284	107.682	1.00 51.33	A	C
	ATOM	700	OE1	GLU	188	10.033	-17.060	106.614	1.00 51.74	A	0
	ATOM	701	OE2	GLU	188	8.465	-16.582	108.081	1.00 52.98	A	0
	ATOM	702	С	GLU	188	7.860	-21.182	108.814	1.00 45.35	A	C
15	MOTA	703	0	GLU	188	7.975	-22.407	108.769	1.00 44.56	A	0
	MOTA	704	N	ASP	189	7.385	-20.544	109.879	1.00 44.44	A	N
	MOTA	705	CA	ASP	189	6.945	-21.271	111.062	1.00 43.61	Α	C
	MOTA	706	CB	ASP	189	6.674	-20.307	112.215	1.00 44.85	Α	C
	MOTA	707	CG	ASP	189		-19.883	112.922	1.00 45.63	A	С
20	MOTA	708	OD1	ASP	189	7.856	-19.099	113.886	1.00 46.80	A	0
	MOTA	709	OD2	ASP	189		-20.339		1.00 47.10	A	0
	MOTA	710	С	ASP	189	5.689	-22.070	110.750	1.00 42.60	A	C
	MOTA	711	0	ASP	189	5.476	-23.142	111.309	1.00 42.20	Α	0
	MOTA	712	N	GLN	190			109.860	1.00 41.71	A	N
25	ATOM	713	CA	GLN	190	3.636	-22.230	109.463	1.00 41.03	A	C
	MOTA	714	CB	GLN	190	2.793	-21.346	108.548	1.00 40.62	A	С
	MOTA	715	CG	GLN	190	2.293	-20.072	109.203	1.00 40.82	Α	С
	MOTA	716	CD	GLN	190			108.348	1.00 40.63	Α	С
00	ATOM	717	OE1	GLN	190			108.590	1.00 41.15	A	0
30	MOTA	718	NE2		190			107.350	1.00 39.87	A	N
	MOTA	719	C	GLN	190			108.733	1.00 40.60	A	C
	ATOM	720	0	GLN	190			108.964	1.00 40.55	A	0
	MOTA	721	N	ILE	191			107.850	1.00 40.63	A	N
0.5	MOTA	722	CA	ILE	191			107.095	1.00 40.39	A	C
35	MOTA	723	CB	ILE	191			106.142	1.00 41.16	A	С
	ATOM	724	CG2		191			105.325	1.00 41.08	A	С
	MOTA	725	CG1		191			105.216	1.00 42.55	Α	С
	ATOM	726	CD1		191		-23.362		1.00 43.94	A	С
40	ATOM	727	С	ILE	191		-25.635		1.00 39.72	Α	C
40	ATOM	728	0	ILE	191		-26.792		1.00 40.14	A	0
	ATOM	729	N	SER	192			108.944	1.00 38.77	A	N
	ATOM	730	CA	SER	192			109.918	1.00 38.58		С
	ATOM	731	CB	SER	192			110.836	1.00 39.73	A	С
15	ATOM	732	OG	SER	192			110.072	1.00 41.62	A	0
45	ATOM	733	C	SER	192			110.760	1.00 36.86	A	С
	ATOM	734	0	SER	192			110.868	1.00 36.31	A	0
	ATOM	735	N	LEU	193			111.353	1.00 35.10	A	Ŋ
	ATOM	736	CA	LEU	193			112.181	1.00 34.68	A	C
50	ATOM	737	CB	LEU	193			112.821	1.00 34.16	A	С
30	ATOM	738	CG	LEU	193			113.887	1.00 34.02	A	C
	ATOM	739		LEU	193			114.445	1.00 33.54	A	C
	ATOM	740		LEU	193			115.005	1.00 33.52	A	C
	MOTA	741	С	LEU	193			111.395	1.00 34.25	A	C
55	MOTA	742	0	LEU	193			111.888	1.00 32.86	A	0
55	ATOM	743	N	LEU	194			110.169	1.00 34.57	A	И
	ATOM	744	CA	LEU	194			109.317	1.00 35.38	A	_
	MOTA	745	CB	LEU	194			108.025	1.00 36.27	A	C
	MOTA	746	CG	LEU	194	0.950	-27.91	. 107.161	1.00 37.99	A	С

-182-

	MOTA	747	CD1	_	194			107.890	1.00 36.63	A	C
	ATOM	748		LEU	194		-27.162		1.00 39.17	A	C
	MOTA	749	С	LEU	194		-29.420		1.00 35.03	A	C
_	ATOM	750	0	LEU	194		-30.470		1.00 34.17	A	0
5	ATOM	751	N	LYS	195		-29.376		1.00 34.97	A	N
	ATOM	752	CA	LYS	195		-30.587		1.00 34.93	Α	C
	ATOM	753	CB	LYS	195	6.491	-30.241	107.796	1.00 36.64	A	C
	MOTA	754	CG	LYS	195		-29.420		1.00 38.77	A	C
	MOTA	755	CD	LYS	195	7.978	-29.272	106.017	1.00 40.24	A	C
10	MOTA	756	CE	LYS	195	8.054	-28.509	104.698	1.00 40.73	A	C
	MOTA	757	NZ	LYS	195	7.263	-29.167	103.615	1.00 42.42	A	N
	ATOM	758	С	LYS	195	5.190	-31.510	109.493	1.00 33.81	A	C
	ATOM	759	0	LYS	195	5.027	-32.729	109.382	1.00 33.63	Α	0
	MOTA	760	N	GLY	196	5.465	-30.921	110.650	1.00 32.20	A	N
15	MOTA	761	CA	GLY	196	5.617	-31.713	111.852	1.00 30.60	A	C
	MOTA	762	C	GLY	196	4.346	-32.292	112.443	1.00 29.37	A	С
	ATOM	763	0	GLY	196	4.400	-33.342	113.085	1.00 28.60	A	0
	ATOM	764	N	ALA	197		-31.648		1.00 27.66	A	N
	ATOM	765	CA	ALA	197	1.958	-32.119	112.804	1.00 26.31	A	C
20	ATOM	766	CB	ALA	197			113.699	1.00 26.25	A	C
	MOTA	767	С	ALA	197			111.919	1.00 25.33	Α	C
	ATOM	768	0	ALA	197			112.427	1.00 24.11	A	Ō
	ATOM	769	N	ALA	198			110.617	1.00 24.59	A	N
	ATOM	770	CA	ALA	198			109.702	1.00 23.71	A	C
25	MOTA	771	CB	ALA	198			108.248	1.00 21.84	A	C
	ATOM	772	С	ALA	198			109.901	1.00 22.64	A	Č
	MOTA	773	0	ALA	198			110.102	1.00 22.27	A	ō
	MOTA	774	N	VAL	199		-35.259		1.00 21.45	A	N
	ATOM	775	CA	VAL	199			109.988	1.00 20.82	A	C
30	ATOM	776	СВ	VAL	199			109.682	1.00 20.86	A	C
	ATOM	777	CG1	VAL	199			110.025	1.00 20.51	A	Ċ
	MOTA	778	CG2		199			108.201	1.00 19.73	A	Č
	ATOM	779	C	VAL	199			111.387	1.00 21.29	A	Ċ
	ATOM	780	0	VAL	199			111.539	1.00 20.92	A	ŏ
35	ATOM	781	N	GLU	200			112.406	1.00 20.35	A	N
	ATOM	782	CA	GLU	200			113.775	1.00 21.19	A	C
	ATOM	783	CB	GLU	200			114.747	1.00 21.68	A	Č
	ATOM	784	CG	GLU	200			114.891	1.00 22.67	A	C
	ATOM	785	CD	GLU	200			115.895	1.00 23.90	A	Č
40	ATOM	786	OE1		200			116.690	1.00 23.20	A	ō
	ATOM	787	OE2		200			115.897	1.00 25.78	A	ō
	MOTA	788	С	GLU	200			113.930	1.00 21.10	A	
	MOTA	789	0	GLU	200	-2.766	-36.802	114.466	1.00 20.46	Α	0
	ATOM	790	N	ILE	201			113.459	1.00 20.78	A	N
45	ATOM	791	CA	ILE	201			113.531	1.00 21.26	A	C
	MOTA	792	СВ	ILE	201			112.901	1.00 21.50	A	Č
	ATOM	793	CG2		201			112.825	1.00 22.57	A	Č
	ATOM	794		ILE	201			113.735	1.00 21.48	Α	C
	ATOM	795	CD1		201			113.133	1.00 21.35	A	C
50	ATOM	796	C	ILE	201			112.806	1.00 21.13	A	Č
	ATOM	797	ō	ILE	201			113.278	1.00 21.64	A	Ö
	ATOM	798	N	CYS	202			111.657	1.00 20.20	A	N
	ATOM	799	CA	CYS	202			110.893	1.00 20.37	A	C
	ATOM	800	СВ	CYS	202			109.585	1.00 20.42	A	C
55	ATOM	801	SG	CYS	202			108.393	1.00 21.08	A	S
	ATOM	802	c	CYS	202			111.694	1.00 18.85	A	c
	ATOM	803	Ō	CYS	202			111.687	1.00 18.40	A	ŏ
	MOTA	804	N	HIS	203			112.384	1.00 18.00	A	N
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WO 2005/019239 PCT/US2004/023092

-183-

	MOTA	805	CA	HIS	203		-39.635		1.00 18.29	A	C
	MOTA	806	CB	HIS	203		-40.312		1.00 17.63	A	C
	MOTA	807	CG	HIS	203		-41.157		1.00 18.10	Α	C
_	MOTA	808	CD2	HIS	203		-40.986		1.00 17.36	Α	С
5	MOTA	809	ND1		203		-42.318		1.00 17.64	A	N
	ATOM	810	CE1	HIS	203	-2.616	-42.825	111.225	1.00 17.59	A	С
	MOTA	811	NE2	HIS	203		-42.035		1.00 17.70	A	N
	MOTA	812	С	HIS	203		-39.255		1.00 18.57	A	C
	MOTA	813	0	HIS	203	-6.586	-40.012	114.724	1.00 17.74	Α	0
10	ATOM	814	N	ILE	204	-5.470	-38.080	114.945	1.00 17.95	Α	N
	MOTA	815	CA	ILE	204	-6.326	-37.634	116.031	1.00 18.97	Α	C
	MOTA	816	CB	ILE	204	-5.867	-36.271	116.595	1.00 18.95	A	С
	MOTA	817		ILE	204		-35.696		1.00 17.63	A	C
	ATOM	818	CG1	ILE	204		-36.436		1.00 17.08	A	C
15	MOTA	819	CD1	ILE	204	-3.990	-35.142	117.913	1.00 16.88	A	C
	MOTA	820	С	ILE	204	-7.754	-37.491	115.490	1.00 19.25	Α	C
	ATOM	821	0	ILE	204			116.111	1.00 19.34	Α	0
	ATOM	822	N	VAL	205			114.327	1.00 19.23	Α	N
	MOTA	823	CA	VAL	205	-9.195	-36.660	113.708	1.00 19.58	A	С
20	MOTA	824	CB	VAL	205	-9.070	-35.782	112.437	1.00 19.63	Α	C
	MOTA	825	CG1	VAL	205	-10.396	-35.756	111.680	1.00 20.05	A	С
	MOTA	826		VAL	205	-8.666	-34.371	112.823	1.00 19.24	A	С
	MOTA	827	С	VAL	205	-9.881	-37.979	113.330	1.00 19.64	Α	C
	MOTA	828	0	VAL	205	-11.078	-38.145	113.545	1.00 19.82	Α	0
25	MOTA	829	N	LEU	206	-9.112	-38.911	112.773	1.00 19.63	A	N
	MOTA	830	CA	LEU	206			112.342	1.00 19.49	A	С
	MOTA	831	CB	LEU	206			111.379	1.00 19.58	Α	С
	ATOM	832	CG	LEU	206	-8.980	-40.934	109.879	1.00 21.14	A	C
	ATOM	833		LEU	206			109.455	1.00 20.56	A	С
30	MOTA	834	CD2	LEU	206			109.094	1.00 20.01	Α	C
	MOTA	835	C	LEU	206			113.469	1.00 18.64	Α	С
	MOTA	836	0	LEU	206			113.242	1.00 18.00	A	0
	MOTA	837	N	ASN	207			114.678	1.00 17.72	A	N
	MOTA	838	CA	ASN	207			115.817	1.00 17.71	A	C
35	ATOM	839	CB	ASN	207			117.089	1.00 16.46	A	C
	ATOM	840	ÇG	ASN	207			118.291	1.00 17.11	A	C
	ATOM	841		ASN	207			119.233	1.00 16.94	A	0
	ATOM	842	ND2		207			118.255	1.00 14.15	A	N
40	MOTA	843	С	ASN	207			116.052	1.00 18.08	A	C
40	MOTA	844	0	ASN	207			116.479	1.00 17.24	A	0
	MOTA	845	N	THR	208			115.782	1.00 17.73	A	N
	ATOM	846	CA	THR	208			115.978	1.00 19.30	A	C
	MOTA	847	СВ	THR	208			115.973	1.00 19.32	Α	C
45	ATOM	848		THR	208			114.875	1.00 20.78	A	0
45	MOTA	849	CG2		208			117.284	1.00 20.86	A	C
	MOTA	850	С	THR	208			114.987	1.00 19.41	A	C
	ATOM	851	0	THR	208			115.150	1.00 19.80	A	0
	ATOM	852	N	THR	209			113.964	1.00 19.05	A	N
EΩ	ATOM	853	CA	THR	209			113.045	1.00 19.58	A	C
50	ATOM	854		THR	209			5 111.608	1.00 19.77	A	C
	ATOM	855		THR	209			111.584	1.00 19.93	A	0
	MOTA	856			209			5 111.073	1.00 20.26	A	C
	MOTA	857		THR	209			3 113.537	1.00 19.57	A	
EE	MOTA	858		THR	209			3 113.079		A	
55	ATOM	859		PHE	210	-12.520		7 114.483		A	
	ATOM	860		PHE	210			5 115.006			_
	ATOM	861		PHE	210			7 115.873			-
	MOTA	862	CG	PHE	210	-9.938	5 -47.35	4 116.129	1.00 19.82	Α	С

-184-

	ATOM	863	CD1		210		-47.948		1.00 19.46	A	С
	MOTA	864	CD2		210		-47.926		1.00 18.74	A	C
	MOTA	865	CE1		210		-49.096		1.00 19.60	A	C
_	MOTA	866		PHE	210		-49.072	117.641	1.00 19.21	A	C
5	MOTA	867	CZ	PHE	210		-49.661		1.00 19.22	A	C
	ATOM	868	C	PHE	210		-47.176	115.810	1.00 21.23	A	C
	ATOM	869	0	PHE	210	-13.639		116.756	1.00 20.44	A	0
	MOTA	870	N	CYS	211	-13.229		115.421	1.00 22.24	A	N
10	MOTA	871 872	CA CB	CYS CYS	211	-14.175	-50.117	116.087	1.00 24.03	A	C
10	MOTA MOTA	873	SG	CYS	211 211	-14.950 -16.182		115.049 115.747	1.00 24.67 1.00 25.21	A	C S
	ATOM	87 4	C	CYS	211	-13.385		117.006	1.00 25.21	A A	C
	ATOM	875	0	CYS	211	-12.508		116.562	1.00 23.56	A	0
	ATOM	876	N	LEU	212		-50.179		1.00 25.72	Α	N
15	ATOM	877	CA	LEU	212		-51.006		1.00 27.59	A	C
	MOTA	878	CB	LEU	212		-50.578		1.00 27.74	A	č
	ATOM	879	CG	LEU	212		-49.185		1.00 28.59	A	c
	ATOM	880	CD1		212		-48.759		1.00 28.93	A	č
	MOTA	881		LEU	212			121.125	1.00 27.26	A	Č
20	ATOM	882	C	LEU	212		-52.489		1.00 29.09	A	C
	ATOM	883	0	LEU	212			119.189	1.00 28.72	A	0
	ATOM	884	N	GLN	213	-14.524	-52.805	118.765	1.00 30.49	Α	N
	ATOM	885	CA	GLN	213	-14.956	-54.181	118.583	1.00 32.47	A	С
	MOTA	886	СВ	GLN	213			118.283	1.00 35.49	A	C
25	MOTA	887	CG	GLN	213	-17.157	-55.523	118.581	1.00 40.38	A	C
	MOTA	888	CD	GLN	213			120.073	1.00 42.74	A	C
	ATOM	889		GLN	213			120.806	1.00 44.72	A	0
	MOTA	890	NE2		213			120.528	1.00 44.13	A	N
20	MOTA	891	C	GLN	213			117.474	1.00 31.71	A	C
30	ATOM	892	0	GLN	213			117.662	1.00 31.33	A	0
	MOTA	893	N	THR	214			116.319	1.00 30.92	A	N
	MOTA	894	CA	THR	214			115.183	1.00 30.21	A	C
	ATOM	895	CB	THR	214			113.898	1.00 30.65	A	C
35	MOTA MOTA	896 897	OG1 CG2		214 214			113.707 113.983	1.00 30.08 1.00 30.64	A	0
00	ATOM	898	CGZ	THR	214			113.983	1.00 30.64	A A	C
	ATOM	899	Ö	THR	214			114.079	1.00 29.04	A	o
	ATOM	900	N	GLN	215			115.625	1.00 29.13	A	N
	ATOM	901	CA	GLN	215			115.454	1.00 29.85	A	C
40	ATOM	902	СВ	GLN	215			115.775	1.00 31.30	Α	c
	ATOM	903	CG	GLN	215			116.476	1.00 35.10	A	Ċ
	ATOM	904	CD	GLN	215			117.919	1.00 36.36	A	Č
	ATOM	905		GLN	215	-9.137	-53.351	118.547	1.00 36.52	Α	0
	ATOM	906	NE2	GLN	215	-7.228	-52.163	118.456	1.00 37.92	Α	N
45	ATOM	907	C	GLN	215	-10.045	-52.300	114.007	1.00 29.28	Α	C
	MOTA	908	0	GLN	215			113.397	1.00 29.33	Α	0
	MOTA	909	N	ASN	216			113.472	1.00 27.92	A	N
	ATOM	910	CA	ASN	216			112.104	1.00 27.75	Α	C
50	MOTA	911	CB	ASN	216			111.276	1.00 29.04	A	C
50	MOTA	912	CG	ASN	216			110.966	1.00 31.13	A	С
	ATOM	913		ASN	216			110.566	1.00 31.15	A	0
	ATOM	914		ASN	216			111.130	1.00 32.04	A	N
	ATOM	915	C	ASN	216			112.109	1.00 26.04	A	C
55	ATOM	916	0	ASN	216			113.079	1.00 25.94	A	0
J	ATOM	917	N	PHE	217 217			111.012 110.868	1.00 24.54	A	
	ATOM ATOM	918 919	CA CB	PHE PHE	217			110.868 110.247	1.00 23.68 1.00 21.91	A A	-
	ATOM	920	CG	PHE	217			3 111.132	1.00 21.91	A	C
	AT OM	220	Ç.G	£11E	21/	-9.6/1	40.723	,	1.00 21.44		_

-185-

5 20 25 30 35 40 45	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	921 922 923 924 925 926 927 928 929 931 932 933 934 935 936 937 938 940 941 942 943 944 945 946	CE1 CE2 CZ CO NCA CB CGCD1 CD2 CO NCA CB SG CO NCA CB CD CD CD CD CD CD CD CD CD CD CD CD CD	PHE PHE PHE PHE PHE LEU LEU LEU LEU CYS CYS CYS CYS CYS GLY GLY	217 217 217 217 217 217 218 218 218 218 218 218 218 219 219 219 219 220 220	-9.127 -7.191 -8.024 -7.057 -12.821 -12.714 -13.976 -15.217 -16.388 -16.185 -17.413 -15.923 -15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640	-47.702 -49.017 -49.316 -50.148 -45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	111.977 111.982 112.825 112.826 109.944 108.778 110.475 109.697 110.591 111.344 112.191 110.346 109.110 109.830 107.798 107.798 107.798 107.502 106.087 104.889	1.00 20.23 1.00 21.42 1.00 21.65 1.00 21.20 1.00 20.69 1.00 23.24 1.00 23.15 1.00 22.85 1.00 22.85 1.00 22.69 1.00 24.13 1.00 24.57 1.00 24.80 1.00 21.34 1.00 20.56 1.00 20.03 1.00 20.03 1.00 21.17 1.00 21.14 1.00 20.85	A A A A A A A A A A A A A A A A A	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
5 2 2 2 3 3 3 3 3 4 4 0 4 5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	923 924 925 926 927 928 929 930 931 932 933 934 935 939 940 941 942 943 944 945	CE1 CE2 CZ CO NCA CB CGCD1 CD2 CO NCA CB SG CO NCA CB CD CD CD CD CD CD CD CD CD CD CD CD CD	PHE PHE PHE PHE LEU LEU LEU LEU CYS CYS CYS CYS CYS GLY GLY	217 217 217 217 218 218 218 218 218 218 219 219 219 219 219 220 220	-7.191 -8.024 -7.057 -12.821 -12.714 -13.976 -15.217 -16.388 -16.185 -17.413 -15.923 -15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-47.603 -45.509 -46.497 -47.677 -48.053 -47.292 -47.702 -49.017 -49.316 -50.148 -45.919 -44.984 -45.805 -44.541 -44.055 -44.667 -44.904	111.982 112.825 112.826 109.944 108.778 110.475 109.697 110.591 111.344 112.191 110.346 109.110 109.830 107.798 107.101 106.399 107.502 106.087 104.889	1.00 21.65 1.00 21.20 1.00 20.69 1.00 23.24 1.00 23.15 1.00 22.85 1.00 22.28 1.00 24.13 1.00 24.57 1.00 24.80 1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.03 1.00 20.03 1.00 21.17 1.00 21.14	A A A A A A A A A A A A A A A A A A A	CCCCCONCCCCCCONCCS
5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	924 925 926 927 928 929 930 931 932 933 934 935 939 940 941 942 943 944 945	CE2 CZ CO NCA CB CGCD1 CD2 CO NCA CB SG CO NCA CB CC CO NCA CB CC CO CO CD CO CO CO CO CO CO CO CO CO CO CO CO CO	PHE PHE PHE LEU LEU LEU LEU CYS CYS CYS CYS CYS GLY GLY	217 217 217 218 218 218 218 218 218 218 219 219 219 219 219 220 220	-8.024 -7.057 -12.821 -12.714 -13.976 -15.217 -16.388 -16.185 -17.413 -15.923 -15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-45.509 -46.497 -47.677 -48.053 -47.292 -47.702 -49.017 -49.316 -50.148 -45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	112.825 112.826 109.944 108.778 110.475 109.697 110.591 111.344 112.191 110.346 109.110 109.830 107.798 107.798 107.101 106.399 107.502 106.087 104.889	1.00 21.20 1.00 20.69 1.00 23.24 1.00 23.15 1.00 22.85 1.00 22.28 1.00 24.13 1.00 24.57 1.00 24.80 1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.03 1.00 20.03 1.00 21.17 1.00 21.14	A A A A A A A A A A A A A A A	CCCONCCCCCCONCCS
 5 10 15 20 25 30 35 40 45 	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	925 926 927 928 929 930 931 932 933 934 935 936 937 940 941 942 943 944 945	CZ C O N CA CB CG CD1 CD2 C O N CA CB SG C O N CA CB C O O C O C O C O C O C O C O C O C	PHE PHE LEU LEU LEU LEU CYS CYS CYS CYS CYS GLY GLY	217 217 218 218 218 218 218 218 218 219 219 219 219 219 220 220	-7.057 -12.821 -12.714 -13.976 -15.217 -16.388 -16.185 -17.413 -15.923 -15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-46.497 -47.677 -48.053 -47.292 -47.702 -49.017 -49.316 -50.148 -45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	112.826 109.944 108.778 110.475 109.697 110.591 111.344 112.191 110.346 109.110 109.830 107.798 107.101 106.399 107.502 106.087 104.889	1.00 20.69 1.00 23.24 1.00 23.15 1.00 22.85 1.00 22.28 1.00 24.13 1.00 24.57 1.00 24.80 1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.03 1.00 20.03 1.00 21.17 1.00 21.14	A A A A A A A A A A A A A A A A A A A	CCCONCCCCCCONCCS
10 20 25 30 35 40 45	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	926 927 928 929 930 931 932 933 934 935 936 937 940 941 942 943 944 945	C O N CA CB CG CD1 CD2 C O N CA CB SG C O N CA C C O N CA C C O N C C C O C C C C C C C C C C C C	PHE PHE LEU LEU LEU LEU CYS CYS CYS CYS CYS GLY GLY	217 218 218 218 218 218 218 218 219 219 219 219 219 220 220	-12.821 -12.714 -13.976 -15.217 -16.388 -16.185 -17.413 -15.923 -15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-47.677 -48.053 -47.292 -47.292 -47.702 -49.017 -49.316 -50.148 -45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	109.944 108.778 110.475 109.697 110.591 111.344 112.191 110.346 109.110 109.830 107.798 107.798 107.101 106.399 107.502 106.087 104.889	1.00 23.24 1.00 23.15 1.00 22.85 1.00 22.28 1.00 24.13 1.00 24.57 1.00 24.80 1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.80 1.00 20.03 1.00 21.17 1.00 21.14	A A A A A A A A A A A A A A A A A A A	CONCCCCCCONCCS
10 15 15 15 15 15 15 15 15 15 15 15 15 15	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	927 928 929 930 931 932 933 934 935 936 937 938 940 941 942 943 944 945	O N CA CB CG CD1 CD2 C O N CA CB SG C O N CA C C O N CA C C O N CA C C O C C C C O C C C C C C C C C C	PHE LEU LEU LEU LEU CYS CYS CYS CYS CYS GLY GLY	217 218 218 218 218 218 218 219 219 219 219 220 220	-12.714 -13.976 -15.217 -16.388 -16.185 -17.413 -15.923 -15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-48.053 -47.292 -47.292 -47.702 -49.017 -49.316 -50.148 -45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	108.778 110.475 109.697 110.591 111.344 112.191 110.346 109.110 109.830 107.798 107.101 106.399 107.502 106.087 104.889	1.00 23.15 1.00 22.85 1.00 22.28 1.00 22.69 1.00 24.13 1.00 24.57 1.00 24.80 1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.03 1.00 20.03 1.00 21.17 1.00 21.14	A A A A A A A A A A A A A A A	CONCCCCCCONCCS
10 15 15 15 15 15 15 15 15 15 15 15 15 15	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	928 929 930 931 932 933 934 935 936 937 938 940 941 942 943 944	N CA CB CG CD1 CD2 C O N CA CB SG C O N CA	LEU LEU LEU LEU LEU CYS CYS CYS CYS CYS CYS GLY GLY	218 218 218 218 218 218 218 219 219 219 219 219 220 220	-13.976 -15.217 -16.388 -16.185 -17.413 -15.923 -15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-47.292 -47.702 -49.017 -49.316 -50.148 -45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	110.475 109.697 110.591 111.344 112.191 110.346 109.110 109.830 107.798 107.101 106.399 107.502 106.087 104.889	1.00 22.85 1.00 22.28 1.00 22.69 1.00 24.13 1.00 24.57 1.00 24.80 1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.03 1.00 20.03 1.00 21.17 1.00 21.14	A A A A A A A A A A A A A A	NCCCCCCONCCS
10 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	929 930 931 932 933 934 935 936 937 938 940 941 942 943 944 945	CA CB CG CD1 CD2 C O N CA CB SG C O N CA C O O	LEU LEU LEU LEU CYS CYS CYS CYS CYS CYS GLY GLY	218 218 218 218 218 218 219 219 219 219 219 220 220	-15.217 -16.388 -16.185 -17.413 -15.923 -15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-47.292 -47.702 -49.017 -49.316 -50.148 -45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	109.697 110.591 111.344 112.191 110.346 109.110 109.830 107.798 107.101 106.399 107.502 106.087 104.889	1.00 22.28 1.00 22.69 1.00 24.13 1.00 24.57 1.00 24.80 1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.80 1.00 20.03 1.00 21.17 1.00 21.14	A A A A A A A A A A	CCCCCCONCCS
10 1 15 2 20 2 30 35 40	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945	CB CG CD1 CD2 C O N CA CB SG C O N CA	LEU LEU LEU LEU CYS CYS CYS CYS CYS CYS GLY GLY	218 218 218 218 218 219 219 219 219 219 220 220	-16.388 -16.185 -17.413 -15.923 -15.478 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-47.702 -49.017 -49.316 -50.148 -45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	110.591 111.344 112.191 110.346 109.110 109.830 107.798 107.101 106.399 107.502 106.087 104.889	1.00 22.69 1.00 24.13 1.00 24.57 1.00 24.80 1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.80 1.00 20.03 1.00 21.17	A A A A A A A	CCCCCOXCCS
15 20 25 30 35 40	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	931 932 933 934 935 936 937 938 939 940 941 942 943 944	CG CD1 CD2 C O N CA CB SG C O N CA	LEU LEU LEU CYS CYS CYS CYS CYS CYS CYS GLY GLY	218 218 218 218 219 219 219 219 219 220 220	-16.185 -17.413 -15.923 -15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-49.017 -49.316 -50.148 -45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	111.344 112.191 110.346 109.110 109.830 107.798 107.101 106.399 107.502 106.087 104.889	1.00 24.13 1.00 24.57 1.00 24.80 1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.80 1.00 20.03 1.00 21.17	A A A A A A	CCCCCOXCCS
15 20 25 30 35 40 45	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	932 933 934 935 936 937 938 939 940 941 942 943 944	CD1 CD2 C O N CA CB SG C O N CA	LEU LEU LEU CYS CYS CYS CYS CYS CYS GLY GLY	218 218 218 218 219 219 219 219 219 220 220	-17.413 -15.923 -15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-49.316 -50.148 -45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	112.191 110.346 109.110 109.830 107.798 107.101 106.399 107.502 106.087 104.889	1.00 24.57 1.00 24.80 1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.80 1.00 20.03 1.00 21.17 1.00 21.14	A A A A A A	CCCCONCCS
15 20 25 30 35 40 45	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	933 934 935 936 937 938 939 940 941 942 943 944	CD2 C O N CA CB SG C O N CA	LEU LEU CYS CYS CYS CYS CYS CYS GLY GLY	218 218 218 219 219 219 219 219 220 220	-15.923 -15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-50.148 -45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	110.346 109.110 109.830 107.798 107.101 106.399 107.502 106.087 104.889	1.00 24.80 1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.80 1.00 20.03 1.00 21.17 1.00 21.14	A A A A A	CCCONCCS
15 20 25 30 35 40 45	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	934 935 936 937 938 939 940 941 942 943 944	C O N CA CB SG C O N CA C O O	LEU LEU CYS CYS CYS CYS CYS GLY GLY GLY	218 219 219 219 219 219 219 219 220 220	-15.478 -15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-45.919 -44.984 -45.805 -44.541 -44.136 -44.055 -44.667 -44.904	109.110 109.830 107.798 107.101 106.399 107.502 106.087 104.889	1.00 21.34 1.00 20.56 1.00 21.05 1.00 20.80 1.00 20.03 1.00 21.17 1.00 21.14	A A A A A	C O N C C S
15202530354045	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	935 936 937 938 939 940 941 942 943 944 945	O N CA CB SG C O N CA C	LEU CYS CYS CYS CYS CYS CYS GLY GLY	218 219 219 219 219 219 219 220 220	-15.830 -15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-44.984 -45.805 -44.541 -44.136 -44.055 -44.667	109.830 107.798 107.101 106.399 107.502 106.087 104.889	1.00 20.56 1.00 21.05 1.00 20.80 1.00 20.03 1.00 21.17 1.00 21.14	A A A A	0 N C C S
20 25 30 35 40	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	936 937 938 939 940 941 942 943 944 945	N CA CB SG C O N CA C	CYS CYS CYS CYS CYS GLY GLY GLY	219 219 219 219 219 219 220 220	-15.305 -15.502 -14.203 -12.762 -16.640 -16.414	-45.805 -44.541 -44.136 -44.055 -44.667 -44.904	107.798 107.101 106.399 107.502 106.087 104.889	1.00 21.05 1.00 20.80 1.00 20.03 1.00 21.17 1.00 21.14	A A A A	N C C s
20 25 30 35 40	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	937 938 939 940 941 942 943 944 945	CA CB SG C O N CA C	CYS CYS CYS CYS CYS GLY GLY	219 219 219 219 219 220 220	-15.502 -14.203 -12.762 -16.640 -16.414	-44.541 -44.136 -44.055 -44.667 -44.904	107.101 106.399 107.502 106.087 104.889	1.00 20.80 1.00 20.03 1.00 21.17 1.00 21.14	A A A	C C S
20 25 30 35 40	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	938 939 940 941 942 943 944 945	CB SG C O N CA C	CYS CYS CYS CYS GLY GLY	219 219 219 219 220 220	-14.203 -12.762 -16.640 -16.414	-44.136 -44.055 -44.667 -44.904	106.399 107.502 106.087 104.889	1.00 20.03 1.00 21.17 1.00 21.14	A A	c s
202530354045	ATOM ATOM ATOM ATOM ATOM ATOM	939 940 941 942 943 944 945	SG C O N CA C	CYS CYS CYS GLY GLY	219 219 219 220 220	-12.762 -16.640 -16.414	-44.055 -44.667 -44.904	107.502 106.087 104.889	1.00 21.17 1.00 21.14	A	S
202530354045	ATOM ATOM ATOM ATOM ATOM	940 941 942 943 944 945	C O N CA C	CYS CYS GLY GLY	219 219 220 220	-16.640 -16.414	-44.667 -44.904	106.087 104.889	1.00 21.14		
25 30 35 40	MOTA ATOM ATOM ATOM	941 942 943 944 945	O N CA C	GLY GLY GLY	219 220 220	-16.414	-44.904	104.889		Α	C
2530354045	ATOM ATOM ATOM	942 943 944 945	N CA C	GLY GLY	220 2 20				1 00 20 05		J
2530354045	ATOM ATOM	943 944 945	CA C O	GLY GLY	220	-17.865	-44 402		1.00 20.03	Α	0
30354045	MOTA	944 945	C	GLY			~~~,474	106.574	1.00 21.18	Α	N
354045		945	0		220	-19.024	-44.612	105.710	1.00 21.35	Α	C
30 35 40 45			-	~	220	-19.104	-46.047	105.222	1.00 21.61	Α	C
30 35 40 45	MOTA	946		GLY	220	-19.079	-46.971	106.025	1.00 21.96	A	0
30 35 40 45	MOTA		N	PRO	221	-19.197	-46.270	103.908	1.00 21.46	A	N
35 40 45	MOTA	947	CD	PRO	221	-19.369	-45.295	102.816	1.00 21.21	Α	С
35 40 45	MOTA	948	CA	PRO	221	-19.273	-47.640	103.402	1.00 22.15	Α	С
35 40 45	MOTA	949	CB	PRO	221	-19.909	-47.451	102.027	1.00 21.42	A	С
35 40 45	MOTA	950	CG	PRO	221	-19.277	-46.164	101.576	1.00 20.84	A	C
35 40 45	MOTA	951	С	PRO	221	-17.893	-48.313	103.320	1.00 22.19	Α	C
35 40 45	MOTA	952	0	PRO	221			102.938	1.00 22.79	Α	0
4045	MOTA	953	N	LEU	222			103.678	1.00 21.79	A	N
40 45	ATOM	954	CA	LEU	222			103.633	1.00 21.31	A	C
40 45	MOTA	955	CB	LEU	222			103.093	1.00 19.09	A	С
40 45	ATOM	956	CG	LEU	222			101.644	1.00 18.95	Α	C
40 45	MOTA	957	CD1		222			101.319	1.00 18.64	A	C
40 45	MOTA	958		LEU	222			100.691	1.00 16.82	A	С
45	MOTA	959	С	LEU	222			104.999	1.00 21.86	A	С
45	MOTA	960	0	LEU	222			106.030	1.00 21.48	A	0
45	ATOM	961	N	ARG	223			104.979	1.00 21.57	A	N
45	MOTA	962	CA	ARG	223			106.175	1.00 22.37	Α	
45	MOTA	963	CB	ARG	223			106.465	1.00 24.98	Α	С
	MOTA	964	CG	ARG	223			107.490	1.00 28.92	A	C
	λπ∩м	965	CD	ARG	223			106.858	1.00 32.82	A	C
	ATOM	966	NE	ARG	223			106.324	1.00 36.01	A	N
	MOTA	967	CZ	ARG	223			105.057	1.00 36.66	A	C
	ATOM ATOM	968	NH1		223			104.167	1.00 36.15	A	N
	ATOM ATOM ATOM		NH2		223			104.677	1.00 36.63	A	N
	ATOM ATOM ATOM	969	C	ARG	223			105.967	1.00 21.18	A	С
	ATOM ATOM ATOM ATOM	970	0	ARG	223			105.070	1.00 20.16	A	0
	ATOM ATOM ATOM ATOM ATOM	970 971		TYR	224			106.782	1.00 18.92	A	N
	ATOM ATOM ATOM ATOM ATOM ATOM	970 971 972	N	TYR	224			106.678	1.00 19.29	A	C
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	970 971 972 973	CA	M1	224			106.716	1.00 17.44	A	C
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	970 971 972 973 974	CA CB	TYR	224			105.604	1.00 17.07	A	C
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	970 971 972 973 974 975	CA CB CG	TYR			-46.908	105./41	1.00 16.45	A	C
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	970 971 972 973 974 975	CA CB CG CD1	TYR TYR	224	4 4 4 4 4	46 050			Α	C
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	970 971 972 973 974 975	CA CB CG CD1 CE1	TYR	224 224 224			104.711	1.00 16.85 1.00 16.10	A	C

-186-

		070	000		004		46 00-				_
	ATOM	979		TYR	224		-46.897		1.00 16.65	A	C
	MOTA	980	CZ	TYR	224		-46.052		1.00 16.90	Α	C
	MOTA	981	OH	TYR	224		-45.234		1.00 16.57	A	0
c	ATOM	982		TYR	224		-50.949		1.00 18.68	A	C
5	MOTA	983	0	TYR	224		-50.713		1.00 18.12	Α	0
	ATOM	984	N	THR	225	-8.543	-51.951	107.516	1.00 17.86	A	N
	MOTA	985	CA	THR	225		-52.894		1.00 18.12	A	C
	MOTA	986	CB	THR	225	-8.322	-54.355	108.091	1.00 16.87	A	C
	MOTA	987	OG1	THR	225	-7.612	-54.637	106.883	1.00 16.75	A	0
10	MOTA	988	CG2	THR	225	-9.803	-54.578	107.848	1.00 15.99	A	C
	MOTA	989	C	THR	225	-6.514	-52.781	108.624	1.00 17.74	A	C
	MOTA	990	0	THR	225		-52.164		1.00 17.42	Α	0
	ATOM	991	N	ILE	226		-53.404		1.00 16.95	A	N
	MOTA	992	CA	ILE	226			109.861	1.00 17.61	A	C
15	ATOM	993	СВ	ILE	226		-53.985		1.00 17.39	A	c
. •	MOTA	994	CG2	ILE	226		-55.476	111.290	1.00 17.55	A	C
	ATOM	995	CG1	ILE	226		-53.713		1.00 17.84	A	c
	ATOM	996	CD1		226		-54.002		1.00 17.04	A	C
	ATOM	997	C	ILE	226		-54.153		1.00 18.23		
20	ATOM	998	Ö	ILE	226		-53.874			A	C
	ATOM	999	Ŋ		227				1.00 16.65	A	0
				GLU			-55.089		1.00 17.96	A	N
	ATOM	1000	CA	GLU	227		-55.840		1.00 19.11	A	C
	ATOM	1001	CB	GLU	227		-56.981		1.00 20.72	A	C
25	ATOM	1002	CG	GLU	227		-58.231		1.00 20.80	Α	C
25	ATOM	1003	CD	GLU	227		-57.975		1.00 21.93	A	C
	ATOM	1004		GLU	227		-57.220		1.00 23.31	A	0
	ATOM	1005	OE2		227		-58.536		1.00 21.48	A	0
	MOTA	1006	С	GLU	227		-54.914		1.00 19.73	A	C
00	MOTA	1007	0	GLU	227		-55.147		1.00 18.85	Α	0
30	MOTA	1008	N	ASP	228		-53.877		1.00 18.55	A	N
	MOTA	1009	CA	ASP	228	-4.371	-52.928	104.533	1.00 19.17	A	C
	MOTA	1010	CB	ASP	228	-5.504	-51.886	104.522	1.00 19.08	A	C
	MOTA	1011	CG	ASP	228	-6.846	-52.496	104.159	1.00 19.07	A	C
	MOTA	1012	OD1	ASP	228	-6.873	-53.316	103.219	1.00 20.93	A	0
35	MOTA	1013	OD2	ASP	228	-7.869	-52.164	104.795	1.00 18.63	A	0
	ATOM	1014	С	ASP	228	-3.012	-52.251	104.691	1.00 18.73	Α	C
	ATOM	1015	0	ASP	228	-2.279	-52.077	103.715	1.00 19.17	A	0
	ATOM	1016	N	GLY	229	-2.672	-51.879	105.922	1.00 18.10	A	N
	ATOM	1017	CA	GLY	229			106.164	1.00 17.50	A	C
40	ATOM	1018	C	GLY	229			105.926	1.00 17.22	A	C
	ATOM	1019	0	GLY	229			105.321	1.00 15.48	A	ō
	ATOM	1020	N	ALA	230	-0.413	-53.461	106.410	1.00 17.33	A	N
	ATOM	1021	CA	ALA	230			106.247	1.00 18.15	A	C
	ATOM	1022	CB	ALA	230			106.987	1.00 16.66	A	c
45	ATOM	1023	C	ALA	230			104.770	1.00 19.00	A	c
	ATOM	1024	ō	ALA	230			104.344	1.00 19.76	A	ŏ
	ATOM	1025	N	ARG	231			103.990	1.00 19.49	A	N
	ATOM	1026	CA	ARG	231			102.566	1.00 19.43	A	C
	ATOM	1027	СВ	ARG	231			101.973	1.00 20.78	A	
50	ATOM	1027	CG	ARG	231			102.524			C
00									1.00 22.44	A	C
	MOTA	1029	CD	ARG	231			102.205	1.00 24.31	A	C
	ATOM	1030	NE	ARG	231			100.783	1.00 26.32	A	N
	ATOM	1031	CZ	ARG	231			100.143	1.00 28.16	A	С
EE	MOTA	1032		ARG	231			100.780	1.00 27.73	Α	N
55	MOTA	1033		ARG	231		-59.233		1.00 30.42	A	N
	MOTA	1034	C	ARG	231			101.721	1.00 19.74	A	C
	MOTA	1035	0	ARG	231			. 100.650	1.00 20.20	A	0
	MOTA	1036	N	VAL	232	0.608	-52 .8 67	102.170	1.00 18.61	Α	N

-187-

	ATOM	1037	CA	VAL	232	1.296	-51.826	101.404	1.00 17.26	A	C
	ATOM	1038	CB	VAL	232	0.569	-50.434	101.462	1.00 17.52	A	C
	ATOM	1039	CG1	VAL	232	-0.855	-50.569	100.919	1.00 17.25	A	C
	ATOM	1040	CG2	VAL	232	0.563	-49.875	102.879	1.00 16.49	A	С
5	ATOM	1041	С	VAL	232	2.748	-51.670	101.852	1.00 17.95	A	C
	ATOM	1042	0	VAL	232		-50.800		1.00 17.18	A	0
	MOTA	1043	N	GLY	233	3.189	-52.510	102.788	1.00 18.73	A	N
	ATOM	1044	CA	GLY	233		-52.442		1.00 19.65	A	C
	MOTA	1045	C	GLY	233		-51.997		1.00 20.28	A	C
10	ATOM	1046	0	GLY	233		-52.078		1.00 20.44	A	0
-	ATOM	1047	N	PHE	234		-51.514		1.00 19.59	A	N
	ATOM	1048	CA	PHE	234		-51.107		1.00 20.47	A	C
	ATOM	1049	СВ	PHE	234		-50.366		1.00 20.71	A	Ċ
	ATOM	1050	CG	PHE	234		-48.963		1.00 21.67	A	C
15	ATOM	1051		PHE	234		-48.602		1.00 21.54	A	C
	ATOM	1052	CD2	PHE	234		-47.996		1.00 22.13	A	Č
	ATOM	1053		PHE	234		-47.291		1.00 23.35	A	Č
	ATOM	1054	CE2		234		-46.681		1.00 23.24	A	C
	ATOM	1055	CZ	PHE	234		-46.328		1.00 23.24	A	C
20	ATOM	1056	C	PHE	234		-52.322		1.00 20.13	A	C
	ATOM	1057	Ö	PHE	234			107.503	1.00 20.13		o
	ATOM	1058	N	GLN	235			107.503	1.00 19.24	A	N
	ATOM	1059	CA	GLN	235			100.334	1.00 20.97	A	C
	ATOM	1060	CB	GLN	235			110.064	1.00 22.42	A	C
25	ATOM	1061	CG	GLN	235			109.069		A	
20	ATOM	1062	CD		235			109.009	1.00 27.92 1.00 30.93	A	C
	ATOM	1062	OE1	GLN	235					A	С 0
	MOTA	1063	NE2		235			109.304 110.703	1.00 33.56	A	
	MOTA	1065	C						1.00 30.93	A	N
30	ATOM			GLN	235			110.494 110.966	1.00 21.69	A	C
30		1066	0	GLN	235			110.966	1.00 20.35	A	0
	ATOM	1067	N	VAL	236				1.00 21.75	A	N
	ATOM	1068	CA	VAL	236			111.850	1.00 20.74	A	C
	ATOM ATOM	1069	CB	VAL	236			112.035	1.00 20.71	A	C
35		1070		VAL	236			113.178	1.00 19.30	A	C
55	MOTA	1071	CG2		236			110.730	1.00 20.83	A	C
	ATOM	1072	C	VAL	236			113.197	1.00 21.19	A	C
	ATOM	1073	0	VAL	236			113.785	1.00 20.57	A	0
	MOTA	1074	N	GLU	237			113.695	1.00 21.62	A	N
40	MOTA	1075	CA	GLU	237			114.981	1.00 23.17	A	C
40	MOTA	1076	CB	GLU	237			115.323	1.00 25.38	A	C
	ATOM	1077	CG	GLU	237			116.535	1.00 29.56	A	C
	ATOM	1078	CD		237			117.002	2.00 02.03	A	_
	ATOM	1079		GLU	237			116.146	1.00 34.48	A	0
45	ATOM	1080		GLU	237			118.227	1.00 33.42	A	0
45	MOTA	1081	C	GLU	237			114.945	1.00 22.30	A	C
	ATOM	1082	0	GLU	237			115.905	1.00 21.24	A	0
	ATOM	1083	N	PHE	238			113.836	1.00 21.77	A	N
	ATOM	1084	CA	PHE	238			113.667	1.00 22.10	A	C
50	ATOM	1085		PHE	238			112.331	1.00 21.91	A	C
50	MOTA	1086		PHE	238			111.954	1.00 22.44	A	C
	MOTA	1087		L PHE	238			112.622	1.00 22.09	A	C
	MOTA	1088		2 PHE	238			110.961	1.00 22.65	A	C
	MOTA	1089		L PHE	238			112.310	1.00 21.36	A	С
ee	ATOM	1090		2 PHE	238			110.636	1.00 22.78	A	С
55	MOTA	1091		PHE	238			l 111.316		A	
	MOTA	1092		PHE	238			2 113.673		A	
	MOTA	1093		PHE	238			1 114.378		A	_
	MOTA	1094	N	LEU	239	2.653	-51.013	3 112.863	1.00 22.09	Α	N

-188-

	MOTA	1095	CA	LEU	239		-51.118		1.00 22.46	A	C
	MOTA	1096	CB	LEU	239		-52.241		1.00 21.56	A	C
	MOTA	1097	CG	LEU	239		-51.905		1.00 23.54	A	С
_	MOTA	1098	CD1		239		-50.519		1.00 22.90	A	С
5	MOTA	1099	CD2		239		-52.977		1.00 21.20	A	C
	MOTA	1100	C	LEU	239		-51.376		1.00 22.41	A	С
	MOTA	1101	0	LEU	239		-50.776		1.00 21.62	A	0
	MOTA	1102	N	GLU	240		-52.262		1.00 22.26	A	N
4.0	MOTA	1103	CA	GLU	240		-52.563		1.00 22.89	A	C
10	MOTA	1104	CB	GLU	240		-53.690		1.00 25.34	A	C
	ATOM	1105	CG	GLU	240		-55.069		1.00 29.77	A	C
	MOTA	1106	CD	GLU	240	-0.189	-55.498	116.294	1.00 33.75	A	С
	MOTA	1107		GLU	240		-54.811		1.00 36.81	A	0
	MOTA	1108	OE2	GLU	240		-56.527		1.00 35.46	A	0
15	ATOM	1109	C	GLU	240	0.705	-51.327	117.151	1.00 21.32	A	C
	MOTA	1110	0	GLU	240	-0.224	-51.081	117.906	1.00 20.62	A	0
	MOTA	1111	N	LEU	241	1.780	-50.554	117.070	1.00 20.96	A	N
	MOTA	1112	CA	LEU	241	1.888	-49.349	117.883	1.00 22.45	Α	C
	MOTA	1113	CB	LEU	241	3.239	-48.664	117.648	1.00 24.05	A	C
20	MOTA	1114	CG	LEU	241	3.466	-47.321	118.363	1.00 26.05	Α	С
	MOTA	1115	CD1	LEU	241	3.433	-47.531	119.877	1.00 27.21	A	C
	MOTA	1116	CD2	LEU	241	4.806	-46.727	117.945	1.00 26.89	A	C
	MOTA	1117	C	LEU	241	0.757	-48.389	117.511	1.00 21.92	A	C
	MOTA	1118	0	LEU	241	0.067	-47.855	118.381	1.00 21.86	Α	0
25	MOTA	1119	N	LEU	242	0.572	-48.194	116.210	1.00 20.84	Α	N
	MOTA	1120	CA	LEU	242	-0.452	-47.303	115.677	1.00 20.79	A	C
	MOTA	1121	CB	LEU	242	-0.433	-47.341	114.146	1.00 19.93	Α	С
	ATOM	1122	CG	LEU	242	-0.682	-46.031	113.392	1.00 21.77	Α	C
	ATOM	1123	CD1	LEU	242	-1.129	-46.358	111.984	1.00 19.10	Α	C
30	ATOM	1124	CD2	LEU	242	-1.729	-45.184	114.085	1.00 21.40	A	C
	ATOM	1125	С	LEU	242	-1.857	-47.667	116.161	1.00 20.42	A	C
	MOTA	1126	0	LEU	242	-2.585	-46.821	116.678	1.00 18.91	A	0
	ATOM	1127	N	PHE	243	-2.231	-48.929	115.981	1.00 20.27	Α	N
	ATOM	1128	CA	PHE	243	-3.545	-49.390	116.386	1.00 20.87	A	C
35	MOTA	1129	CB	PHE	243	-3.828	-50.766	115.775	1.00 21.22	Α	C
	MOTA	1130	CG	PHE	243	-4.211	-50.704	114.309	1.00 21.05	Α	C
	MOTA	1131	CD1	PHE	243	-3.316	-50.212	113.359	1.00 19.68	Α	C
	ATOM	1132	CD2	PHE	243	-5.478	-51.092	113.893	1.00 19.34	A	C
	MOTA	1133	CE1	PHE	243	-3.678	-50.104	112.022	1.00 20.59	Α	C
40	MOTA	1134	CE2	PHE	243			112.558	1.00 19.75	Α	C
	MOTA	1135	CZ	PHE	243	-4.950	-50.492	111.621	1.00 20.16	Α	C
	ATOM	1136	C	PHE	243			117.899	1.00 21.36	Α	C
	MOTA	1137	0	PHE	243	-4.855	-49.217	118.385	1.00 20.70	Α	0
	ATOM	1138	N	HIS	244			118.644	1.00 21.51	A	N
45	MOTA	1139	CA	HIS	244	-2.747	-49.586	120.101	1.00 22.59	Α	C
	ATOM	1140	CB	HIS	244	-1.448	-50.061	120.757	1.00 24.95	Α	С
	MOTA	1141	CG	HIS	244	-1.424	-49.877	122.245	1.00 27.50	Α	С
	MOTA	1142	CD2	HIS	244			. 123.252	1.00 28.29	Α	C
	ATOM	1143	ND1	. HIS	244	-1.033	-48.698	122.846	1.00 28.64	A	N
50	MOTA	1144	CEI	. HIS	244	-1.148	-48.814	124.157	1.00 29.14	Α	C
	MOTA	1145	NE	HIS	244			124.430	1.00 29.46	A	N
	MOTA	1146	C	HIS	244			120.503	1.00 21.62	Α	C
	ATOM	1147	0	HIS	244			121.394	1.00 21.60	A	0
	MOTA	1148	N	PHE	245			119.844	1.00 20.43	A	
55	MOTA	1149		PHE	245			120.106		Α	
	MOTA	1150		PHE	245			119.173		A	C
	MOTA	1151		PHE	245			119.121		A	
	ATOM	1152	CD:	L PHE	245	-1.755	-42.606	5 120.122	1.00 20.84	A	С

-189-

	MOTA	1153	CD2	PHE	245	-2.957	-43.041	118.102	1.00 20.72	A	C
	MOTA	1154	CE1	PHE	245	-2.206	-41.284	120.113	1.00 19.78	A	C
	ATOM	1155	CE2	PHE	245		-41.721		1.00 21.00	A	C
_	MOTA	1156	CZ	PHE	245		-40.844		1.00 20.53	A	C
5	MOTA	1157	С	PHE	245	-4.033	-45.446	119.873	1.00 19.25	A	C
	MOTA	1158	0	PHE	245	-4.676	-44.833	120.721	1.00 19.06	A	0
	MOTA	1159	N	HIS	246	-4.564	-45.844	118.722	1.00 19.01	Α	N
	ATOM	1160	ÇA	HIS	246	-5.954	-45.546	118.400	1.00 19.09	Α	C
_	MOTA	1161	CB	HIS	246	-6.268	-45.962	116.953	1.00 18.50	A	C
10	ATOM	1162	CG	HIS	246	-5.954	-44.898	115.944	1.00 18.48	A	C
	MOTA	1163	CD2	HIS	246	-4.970	-44.805	115.018	1.00 18.21	A	C
	MOTA	1164	ND1	HIS	246	-6.665	-43.719	115.863	1.00 18.52	Α	N
	MOTA	1165	CE1	HIS	246	-6.130	-42.945	114.935	1.00 17.66	Α	C
	ATOM	1166	NE2	HIS	246	-5.100	-43.581	114.407	1.00 18.46	Α	N
15	ATOM	1167	С	HIS	246	-6.939	-46.185	119.377	1.00 18.38	Α	C
	MOTA	1168	0	HIS	246	-7.899	-45.550	119.801	1.00 18.13	A	0
	ATOM	1169	N	GLY	247	-6.704	-47.436	119.739	1.00 19.24	A	N
	ATOM	1170	CA	GLY	247			120.680	1.00 19.94	A	C
	ATOM	1171	С	GLY	247	-7.567	-47.385	122.022	1.00 20.61	A	C
20	ATOM	1172	0	GLY	247	-8.615	-47.103	122.602	1.00 20.87	A	0
	MOTA	1173	N	THR	248			122.511	1.00 19.95	A	N
	ATOM	1174	CA	THR	248			123.793	1.00 20.64	A	C
	MOTA	1175	СВ	THR	248			124.144	1.00 21.09	A	C
	ATOM	1176	OG1	THR	248			124.116	1.00 21.47	A	0
25	MOTA	1177	CG2		248			125.534	1.00 18.96	A	C
	ATOM	1178	C	THR	248			123.814	1.00 20.66	A	C
	ATOM	1179	0	THR	248	-7.642	-44.736	124.766	1.00 20.22	A	0
	ATOM	1180	N	LEU	249	-6.725	-44.270	122.761	1.00 21.23	A	N
	ATOM	1181	CA	LEU	249			122.674	1.00 21.39	A	C
30	ATOM	1182	СВ	LEU	249			121.471	1.00 21.91	A	C
	ATOM	1183	CG	LEU	249			121.301	1.00 22.61	A	C
	MOTA	1184	CD1	LEU	249			122.494	1.00 23.51	Α	C
	ATOM	1185		LEU	249			120.014	1.00 22.87	A	C
	ATOM	1186	С	LEU	249			122.569	1.00 20.82	Α	C
35	MOTA	1187	0	LEU	249			123.152	1.00 19.80	A	0
	MOTA	1188	N	ARG	250			121.828	1.00 21.20	A	N
	ATOM	1189	CA	ARG	250	-10.816	-44.185	121.644	1.00 21.98	Α	C
	ATOM	1190	СВ	ARG	250			120.573	1.00 21.92	Α	C
	ATOM	1191	CG	ARG	250	-12.563	-45.341	120.158	1.00 21.63	Α	C
40	ATOM	1192	CD	ARG	250	-12.994	-44.086	119.412	1.00 24.25	Α	С
	ATOM	1193	NE	ARG	250	-13.967	-44.395	118.368	1.00 25.98	Α	N
	ATOM	1194	CZ	ARG	250	-15.285	-44.293	118.503	1.00 27.08	A	C
	ATOM	1195	NH1	ARG	250	-15.813	-43.874	119.644	1.00 27.73	A	N
	ATOM	1196	NH2	ARG	250	-16.077	-44.637	117.495	1.00 27.60	A	
45	ATOM	1197	C	ARG	250	-11.532	-44.580	122.936	1.00 22.80	Α	C
	ATOM	1198	0	ARG	250	-12.645	-44.126	123.194	1.00 22.12	A	
	ATOM	1199	N	LYS	251	-10.893	-45.431	123.735	1.00 23.54	Α	
	ATOM	1200	CA	LYS	251	-11.471	-45.890	124.997	1.00 24.94	Α	
	ATOM	1201	CB	LYS	251	-10.576	-46.944	125.650	1.00 25.92	Α	
50	MOTA	1202	CG	LYS	251	-10.575	-48.298	124.961	1.00 29.26	Α	
	ATOM	1203	CD	LYS	251	-9.656	-49.271	125.690	1.00 30.89	Α	
	MOTA	1204	CE	LYS	251			124.889	1.00 33.42	A	
	ATOM	1205	NZ	LYS	251			125.462	1.00 35.04	Α	
	MOTA	1206	С	LYS	251			125.992	1.00 25.07		
55	ATOM	1207	0	LYS	251			126.932			
	ATOM	1208	N	LEU	252			125.793		A	
	ATOM	1209		LEU	252			126.685			
	MOTA	1210		LEU	252			126.503			

WO 2005/019239 PCT/US2004/023092

-190-

	MOTA	1211		LEU	252		-42.172		1.00 24.00		C
	ATOM	1212	CD1		252		-41.176		1.00 22.17	A	C
	MOTA	1213	CD2		252		-42.599		1.00 21.31	A	C
6	ATOM	1214		LEU	252	-12.457			1.00 26.07	A	C
5	MOTA	1215		LEU	252	-12.822			1.00 25.67	A	0
	ATOM	1216		GLN	253	-13.165			1.00 27.09	A	N
	MOTA	1217		GLN	253	-14.454			1.00 28.60	A	C
	ATOM	1218		GLN	253	-15.498			1.00 30.52	A	C
40	MOTA	1219		GLN	253	-15.871			1.00 34.58	A	C
10	MOTA	1220		GLN	253	-16.676			1.00 37.32	A	C
	MOTA	1221	OE1		253	-17.588			1.00 38.93	A	0
	ATOM	1222	NE2		253	-16.341			1.00 38.76	A	И
	MOTA	1223	C	GLN	253			125.246	1.00 28.46	A	C
45	ATOM	1224	0	GLN	253			125.986	1.00 28.32	A	0
15	ATOM	1225	N	LEU	254			124.494	1.00 27.65	A	N
	MOTA	1226	CA	LEU	254			124.510	1.00 27.11	A	C
	ATOM	1227	CB	LEU	254			123.821	1.00 25.42	A	C
	ATOM	1228	CG	LEU	254			124.384	1.00 24.68	A	C
20	ATOM	1229	CD1		254			123.621	1.00 23.56	A	C
20	MOTA	1230		LEU	254			125.867	1.00 23.28	A	C
	ATOM	1231	C	LEU	254			123.817	1.00 27.57	A	C
	ATOM	1232	0	LEU	254			122.974	1.00 26.67	A	0
	MOTA	1233	N	GLN	255			124.176	1.00 28.10	A	N
25	ATOM	1234	CA	GLN	255			123.562	1.00 29.49	A	C
25	ATOM	1235	CB	GLN	255			124.616	1.00 31.52	A	C
	MOTA	1236	CG	GLN	255			125.810	1.00 35.22 1.00 38.55	A A	C
	MOTA	1237	CD	GLN	255			126.791			0
	MOTA	1238		GLN	255			127.185	1.00 39.64 1.00 40.55	A	N
30	MOTA	1239	NE2		255			127.199	1.00 40.33	A A	C
30	MOTA	1240	C	GLN	255			122.496	1.00 28.44	A	0
	MOTA	1241	0	GLN	255 256			122.594	1.00 28.49	A	И
	ATOM	1242	N CA	GLU GLU	256			2 120.405	1.00 28.54	A	C
	ATOM	1243			256			119.607	1.00 20.34	A	C
35	ATOM	1244 1245	CB	GLU GLU	256			119.007	1.00 33.85	A	C
33	MOTA MOTA	1245	CD	GLU	256			3 117.304	1.00 35.60	A	C
	ATOM	1247	OE1		256			117.567	1.00 37.88	A	ŏ
	ATOM	1247	OE2		256			116.174	1.00 37.00	A	ŏ
	ATOM	1249	C	GLU	256			3 120.848	1.00 27.93	A	č
40	ATOM	1250	Ö	GLU	256			3 120.319	1.00 27.24	A	ŏ
40	ATOM	1251	N	PRO	257			3 121.813	1.00 28.04	Α	Ŋ
	ATOM	1252		PRO	257			2 122.517	1.00 28.01	A	C
	ATOM	1253	CA	PRO	257			2 122.254	1.00 27.60	A	C
	MOTA	1254		PRO	257			1 123.371	1.00 28.41	A	C
45	ATOM	1255		PRO	257			1 123.795	1.00 29.41	A	
	ATOM	1256		PRO	257			1 122.698	1.00 26.72	Α	Č
	MOTA	1257		PRO	257			7 122.436	1.00 27.19	A	Ō
	ATOM	1258		GLU	258			3 123.357	1.00 25.36	A	
	ATOM	1259		GLU	258			3 123.818	1.00 24.44	Α	
50	MOTA	1260		GLU	258			7 124.813		A	
	ATOM	1261		GLU	258			4 126.004		A	
	MOTA	1262		GLU	258			6 126.911		Α	
	MOTA	1263		L GLU	258			8 126.397			
	ATOM	1264		2 GLU	258			3 128.143			
55	ATOM	1265		GLU				6 122.637			
	MOTA	1266		GLU				9 122.634			
	MOTA	1267		TYR				7 121.634			
	ATOM	1268						4 120.446			
						+					

-191-

	MOTA	1269	CB	TYR	259	-11.091			1.00 21.08	A	C
	MOTA	1270	CG	TYR	259	-11.261			1.00 21.43	A	C
	MOTA	1271	CD1		259	-10.198			1.00 21.24	A	C
_	MOTA	1272	CE1		259	-10.365			1.00 19.51	A	C
5	MOTA	1273	CD2	TYR	259	-12.493			1.00 20.98	A	C
	MOTA	1274	CE2	TYR	259	-12.672			1.00 21.07	A	C
	MOTA	1275	CZ	TYR	259	-11.601			1.00 19.86	A	C
	MOTA	1276	OH	TYR	259			120.006	1.00 18.11	A	0
	MOTA	1277	С	TYR	259			119.723	1.00 22.33	Α	C
10	MOTA	1278	0	TYR	259			119.295	1.00 21.92	A	0
	MOTA	1279	N	VAL	260			119.575	1.00 22.03	A	N
	MOTA	1280	CA	VAL	260			118.877	1.00 23.22	A	C
	MOTA	1281	CB	VAL	260			118.626	1.00 24.49	A	С
	MOTA	1282		VAL	260			118.451	1.00 26.18	A	C
15	ATOM	1283		VAL	260			117.372	1.00 24.67	A	C
	MOTA	1284	С	VAL	260			119.590	1.00 22.97	Α	С
	ATOM	1285	0	VAL	260			118.937	1.00 22.35	Α	0
	MOTA	1286	N	LEU	261			120.916	1.00 23.08	A	N
00	ATOM	1287	CA	LEU	261			121.679	1.00 24.42	A	C
20	MOTA	1288	CB	LEU	261			123.145	1.00 24.90	A	С
	MOTA	1289	CG	LEU	261			123.411	1.00 24.74	A	С
	MOTA	1290		LEU	261			124.808	1.00 25.84	A	С
	ATOM	1291		LEU	261			123.235	1.00 24.89	A	C
05	MOTA	1292	С	LEU	261			121.576	1.00 24.56	A	C
25	MOTA	1293	0	LEU	261			121.469	1.00 24.62	A	0
	MOTA	1294	N	LEU	262			121.602	1.00 24.08	Α	N
	MOTA	1295	CA	LEU	262			121.473	1.00 24.35	A	C
	ATOM	1296	СВ	LEU	262			121.558	1.00 25.52	A	C
20	ATOM	1297	CG	LEU	262			122.018	1.00 26.64	A	С
30	MOTA	1298		LEU	262			123.404	1.00 26.40	A	C
	MOTA	1299		LEU	262			122.044	1.00 26.95	A	С
	MOTA	1300	C	LEU	262			120.112	1.00 23.84	A	C
	MOTA	1301	Ο.	LEU	262			120.009	1.00 23.68	A	0
25	MOTA	1302	N	ALA	263			119.071	1.00 22.30	A	N
35	ATOM	1303	CA	ALA	263			117.749	1.00 22.57	A	C
	ATOM	1304	CB	ALA	263			116.710	1.00 21.76	A	C
	ATOM	1305	C	ALA	263			117.779	1.00 22.78	A	C
	ATOM	1306	0	ALA	263			117.186	1.00 22.16	A	0
40	ATOM	1307	N	ALA	264			118.470	1.00 22.57	A	N
40	ATOM	1308	CA	ALA	264			118.586 119.332	1.00 24.00	A	C
	ATOM ATOM	1309 1310	CB C	ALA ALA	264 264			119.332	1.00 23.05 1.00 24.41	A	C
			_		264			119.302		A	_
	MOTA	1311 1312	0	ALA	265			120.312	1.00 24.83 1.00 25.02	A A	0
45	MOTA	1312	N	MET	265			120.312	1.00 25.02		N
70	ATOM ATOM	1313	CA CB	MET MET	265			121.035	1.00 25.93	A A	C
		1314	CG	MET	265			123.415	1.00 20.79	A	C
	ATOM	1315			265			123.413	1.00 27.47	A	S
	MOTA MOTA	1317	SD CE	MET MET	265			125.669	1.00 23.87	A	C
50		1318	CE	MET	265			120.177	1.00 27.34	A	C
30	ATOM	1319	0		265			120.177	1.00 26.21	A	0
	ATOM ATOM	1320	N	MET ALA	266			119.314	1.00 25.89	A	
	ATOM	1321	CA	ALA	266			3 118.417	1.00 25.79	A	
	ATOM	1321	CB	ALA	266			3 117.700	1.00 24.34	A	
55	ATOM	1322	СВ	ALA	266			5 117.700	1.00 26.44	A	
55	ATOM	1323		ALA	266			2 117.402	1.00 25.58	A	
	ATOM	1324		LEU	267			9 116.936	1.00 25.38	A	
		1325		LEU	267			l 115.968	1.00 20.30	A	
	MOTA	1320	CA	TEO	20/	0.041	20.40.	. 113.300	1.00 29.21	-	C

-192-

	MOTA	1327	CB	LEU	267		-27.636		1.00 28.28	A	C
	ATOM	1328	CG	LEU	267	-1.322	-27.086	114.116	1.00 28.22	Α	C
	ATOM	1329	CD1		267	-2.153	-25.815	114.151	1.00 26.62	A	C
	MOTA	1330	CD2	LEU	267	0.040	-26.797	113.520	1.00 27.55	A	C
5	MOTA	1331	С	LEU	267	1.051	-27.405	116.541	1.00 30.31	Α	C
	ATOM	1332	0	LEU	267		-27.195		1.00 30.73	A	0
	ATOM	1333	N	PHE	268		-26.795		1.00 31.98	A	N
	ATOM	1334	CA	PHE	268		-25.817		1.00 34.42	A	C
	ATOM	1335	СВ	PHE	268			119.065	1.00 33.07	A	č
10	ATOM	1336	CG	PHE	268			118.209	1.00 33.01	A	Č
. •	MOTA	1337		PHE	268			118.224	1.00 33.01		C
	ATOM	1338		PHE	268			117.356	1.00 31.34	A	C
	ATOM	1339	CE1		268			117.330		A	
		1340	CE2		268				1.00 31.94	A	C
15	ATOM			PHE				116.527	1.00 32.75	A	C
15	ATOM	1341	CZ	PHE	268			116.551	1.00 32.01	A	C
	ATOM	1342	C	PHE	268			119.171	1.00 35.98	A	C
	ATOM	1343	0	PHE	268			120.393	1.00 36.42	A	0
	MOTA	1344	N	SER	269			118.537	1.00 38.74	Α	N
00	MOTA	1345	CA	SER	269			119.244	1.00 41.31	A	C
20	MOTA	1346	CB	SER	269			118.743	1.00 41.54	Α	C
	MOTA	1347	OG	SER	269			118.970	1.00 43.06	A	0
	MOTA	1348	C	SER	269	6.026	-26.834	118.969	1.00 42.81	A	C
	MOTA	1349	0	SER	269	6.505	-26.782	117.840	1.00 43.23	A	0
	MOTA	1350	N	PRO	270	6.564	-26.171	120.002	1.00 44.83	Α	N
25	ATOM	1351	CD	PRO	270	6.116	-26.232	121.406	1.00 44.95	A	C
	ATOM	1352	CA	PRO	270	7.758	-25.326	119.873	1.00 46.18	A	C
	MOTA	1353	СВ	PRO	270			121.259	1.00 45.92	A	C
	ATOM	1354	CG	PRO	270			122.156	1.00 45.81	A	C
	ATOM	1355	C	PRO	270			119.452	1.00 47.67	A	Č
30	ATOM	1356	ō	PRO	270			118.935	1.00 48.27	A	ŏ
	ATOM	1357	N	ASP	271			119.672	1.00 48.67	A	N
	ATOM	1358	CA	ASP	271			119.321	1.00 49.58	A	C
	ATOM	1359	СВ	ASP	271			120.409	1.00 50.08	A	C
	ATOM	1360	CG	ASP	271			120.403	1.00 50.89	A	C
35	ATOM	1361	OD1		271			120.767	1.00 50.89	A	0
•	ATOM	1362	OD2		271			120.767	1.00 51.40	A	0
	ATOM	1363	C	ASP	271			117.950	1.00 50.08		C
					271					A	
	MOTA	1364	0	ASP	272			117.644	1.00 50.01	A	0
40	MOTA	1365	N	ARG					1.00 50.50	A	N
70	MOTA	1366	CA	ARG	272			115.784	1.00 51.11	Α	C
	ATOM	1367	CB	ARG	272			115.126	1.00 50.35	A	C
	ATOM	1368	CG	ARG	272			114.325	1.00 49.50	A	C
	ATOM	1369	CD	ARG	272			115.161	1.00 48.07	A	С
AE	ATOM	1370	NE	ARG	272			115.405	1.00 47.04	A	N
45	ATOM	1371	CZ	ARG	272			115.873	1.00 45.93	Α	C
	MOTA	1372		ARG	272			116.154	1.00 45.21	A	N
	MOTA	1373		ARG	272			116.062	1.00 44.85	A	N
	MOTA	1374	C	ARG	272			115.005	1.00 51.77	A	С
	MOTA	1375	0	ARG	272	10.674	-27.271	115.015	1.00 52.46	Α	0
50	MOTA	1376	N	PRO	273			114.317	1.00 52.32	Α	N
	MOTA	1377	CD	PRO	273			114.035	1.00 52.48	Α	C
	MOTA	1378	CA	PRO	273	12.186	-29.020	113.552	1.00 52.55	Α	C
	MOTA	1379	CB	PRO	273	12.567	-30.337	7 112.876	1.00 52.49	A	С
	MOTA	1380	CG	PRO	273			112.706	1.00 52.55	Α	С
55	ATOM	1381	С	PRO				112.550	1.00 52.78	A	C
	ATOM	1382	0	PRO				3 111.628	1.00 52.86	A	
	ATOM	1383	Ŋ	GLY				5 112.742	1.00 52.71	Α	
	ATOM	1384	CA	GLY				3 111.831	1.00 52.86	A	
	011	204		J 1	2 /3	~~. 001	. 23.000		1.00 32.00	-	C

-193-

	ATOM	1385	С	GLY	274	11 921	-24.428	112 306	1.00 53.31	A	С
	ATOM	1386		GLY	274		-23.448		1.00 52.74		Ö
	ATOM	1387		VAL	275		-24.451		1.00 52.74	A	N
				VAL			-23.294			A	
5	MOTA	1388			275				1.00 54.72	A	C
5	MOTA	1389		VAL	275		-23.653		1.00 54.41	A	C
	ATOM	1390	CG1		275		-24.806		1.00 54.40	A	C
	MOTA	1391	CG2		275		-24.010		1.00 54.73	A	C
	MOTA	1392		VAL	275			114.391	1.00 55.42	Α	C
	MOTA	1393	0	VAL	275	12.793	-22.376	114.694	1.00 55.34	A	0
10	MOTA	1394	N	THR	276	11.103	-20.928	114.341	1.00 56.25	A	N
	ATOM	1395	CA	THR	276	11.888	-19.738	114.657	1.00 57.04	A	C
	ATOM	1396	CB	THR	276	12.019	-18.806	113.428	1.00 57.12	A	C
	ATOM	1397	0G1	THR	276	10.728	-18.310	113.054	1.00 57.58	A	0
	ATOM	1398	CG2	THR	276	12.624			1.00 56.94	A	C
15	ATOM	1399	C	THR	276		-18.958	115.810	1.00 57.44	A	C
	ATOM	1400	Ö	THR	276				1.00 57.90	A	ŏ
	ATOM	1401	N	GLN	277				1.00 57.58	A	N
	ATOM	1402	CA	GLN	277				1.00 57.56	A	C
	ATOM	1403	CB	GLN	277			116.453	1.00 57.36		C
20		1404	CG						1.00 57.98	A	C
20	ATOM			GLN	277					A	
	ATOM	1405	CD OP1	GLN	277			115.683	1.00 59.41	A	С
	ATOM	1406	OE1		277		-15.444		1.00 60.10	A	0
	ATOM	1407	NE2	GLN	277			115.171	1.00 59.47	A	N
OF	MOTA	1408	С	GLN	277			118.125	1.00 57.42	A	C
25	MOTA	1409	0	GLN	277			118.629	1.00 57.26	A	0
	ATOM	1410	N	ARG	278			118.531	1.00 57.27	Α	N
	ATOM	1411	CA	ARG	278			119.585	1.00 57.49	A	С
	ATOM	1412	CB	ARG	278			119.951	1.00 58.82	Α	C
	ATOM	1413	CG	ARG	278	11.208	-22.952	120.705	1.00 60.52	A	C
30	MOTA	1414	CD	ARG	278	12.581	-23.453	121.124	1.00 62.18	Α	C
	ATOM	1415	NE	ARG	278	12.567	-24.877	121.465	1.00 63.94	A	N
	ATOM	1416	CZ	ARG	278		-25.415		1.00 64.51	Α	C
	ATOM	1417	NH1		278			122.697	1.00 64.55	A	N
	ATOM	1418		ARG	278			123.328	1.00 64.96	A	N
35	ATOM	1419	С	ARG	278			120.851	1.00 56.92	Α	C
	ATOM	1420	ŏ	ARG	278			121.380	1.00 56.95	A	ŏ
	ATOM	1421	N	ASP	279			121.344	1.00 56.06	A	Ŋ
	ATOM	1422	CA	ASP	279			122.551	1.00 55.37	A	C
	ATOM	1423	CB	ASP	279			122.990	1.00 56.68	A	C
40	ATOM	1424	CG	ASP	279			123.419	1.00 57.63		
70										A	C
	ATOM	1425		ASP ASP	279			122.547		A	0
	ATOM	1426			279				1.00 58.07	A	0
	ATOM	1427	C	ASP	279			122.338	1.00 54.14	A	C
AE	ATOM	1428	0	ASP	279			123.156	1.00 53.64	A	0
45	MOTA	1429	N	GLU	280			121.235	1.00 52.98	Α	Ŋ
	MOTA	1430		GLU	280			120.918	1.00 51.96	Α	C
	ATOM	1431	CB	GLU	280			119.598	1.00 52.88	Α	
	MOTA	1432	CG	GLU	280			7 119.329	1.00 54.43	Α	C
	ATOM	1433	CD	GLU	280			3 117.951	1.00 55.52	Α	C
50	ATOM	1434	OE1	GLU	280	5.204	-14.875	5 117.570	1.00 56.15	Α	0
	MOTA	1435	OE2	GLU	280	3.255	-15.834	1 117.252	1.00 55.94	Α	0
	MOTA	1436	C	GLU	280	4.908	-18.898	3 120.821	1.00 50.62	Α	
	MOTA	1437		GLU	280			7 121.470	1.00 50.58	Α	
	ATOM	1438		ILE	281			7 120.004	1.00 49.04	A	
55	ATOM	1439		ILE	281			3 119.815	1.00 47.41	A	
	ATOM	1440		ILE	281			7 118.764	1.00 46.53	A	
	ATOM	1441		ILE	281			9 118.655	1.00 45.22	A	
	ATOM	1442		ILE				2 117.408	1.00 45.56	A	
	MION	1442	CG1	. TUE	201	3.3/6	, -21.202	. TT1.400	T'00 43'30	A	C

-194-

	MOTA	1443	CD1	ILE	281			116.326	1.00 45.01	A	С
	MOTA	1444	C	ILE	281	4.533	-21.886	121.131	1.00 47.29	A	C
	MOTA	1445	0	ILE	281	3.525	-22.549	121.383	1.00 46.81	A	0
_	MOTA	1446	N	ASP	282			121.965	1.00 46.94	A	N
5	MOTA	1447	CA	ASP	282			123.260	1.00 46.55	A	C
	MOTA	1448	CB	ASP	282	6.946	-22.311	123.926	1.00 47.68	Α	C
	MOTA	1449	CG	ASP	282	7.098	-23.166	125.170	1.00 48.85	A	С
	MOTA	1450	OD1	ASP	282	6.921	-24.402	125.082	1.00 49.57	A	0
_	MOTA	1451	OD2	ASP	282	7.402	-22.602	126.242	1.00 49.92	A	0
10	MOTA	1452	C	ASP	282			124.144	1.00 45.75	A	C
	MOTA	1453	0	ASP	282	3.847	-22.583	124.934	1.00 45.36	A	0
	MOTA	1454	N	GLN	283	4.226	-20.576	124.000	1.00 45.11	A	N
	ATOM	1455	CA	GLN	283	3.181	-19.904	124.770	1.00 45.13	Α	C
	MOTA	1456	CB	GLN	283	3.256	-18.387	124.563	1.00 46.75	A	C
15	MOTA	1457	CG	GLN	283	2.563	-17.534	125.637	1.00 50.09	A	C
	ATOM	1458	CD	GLN	283	1.092	-17.879	125.849	1.00 52.42	Α	C
	MOTA	1459	OE1	GLN	283	0.754	-18.757	126.649	1.00 54.11	A	0
	MOTA	1460	NE2	GLN	283	0.210	-17.189	125.129	1.00 53.63	Α	N
	ATOM	1461	С	GLN	283	1.821	-20.423	124.292	1.00 43.58	Α	C
20	MOTA	1462	0	GLN	283	0.929	-20.680	125.099	1.00 43.49	Α	0
	ATOM	1463	N	LEU	284	1.664	-20.573	122.979	1.00 42.02	A	N
	MOTA	1464	CA	LEU	284	0.409	-21.079	122.428	1.00 40.90	A	C
	MOTA	1465	CB	LEU	284	0.438	-21.086	120.892	1.00 40.60	A	C
	ATOM	1466	CG	LEU	284	0.221	-19.783	120.110	1.00 40.12	Α	С
25	ATOM	1467	CD1	LEU	284	-0.648	-18.833	120.918	1.00 39.50	Α	C
	MOTA	1468	CD2	LEU	284	1.551	-19.146	119.789	1.00 40.64	Α	C
	MOTA	1469	С	LEU	284	0.140	-22.491	122.934	1.00 39.59	Α	C
	MOTA	1470	0	LEU	284	-0.986	-22.825	123.292	1.00 39.24	Α	0
	MOTA	1471	N	GLN	285	1.180	-23.318	122.950	1.00 39.22	A	N
30	MOTA	1472	CA	GLN	285	1.070	-24.688	123.433	1.00 38.77	Α	C
	MOTA	1473	CB	GLN	285	2.454	-25.344	123.452	1.00 39.75	Α	C
	ATOM	1474	CG	GLN	285	2.497	-26.740	124.049	1.00 42.43	Α	C
	MOTA	1475	CD	GLN	285	1.934	-27.788	123.117	1.00 43.45	Α	C
	MOTA	1476	OE1	GLN	285	0.771	-27.728	122.730	1.00 45.03	A	0
35	ATOM	1477	NE2	GLN	285	2.763	-28.757	122.747	1.00 44.86	A	N
	ATOM	1478	С	GLN	285	0.487	-24.653	124.843	1.00 37.86	A	C
	MOTA	1479	0	GLN	285	-0.501	-25.323	125.138	1.00 37.02	Α	0
	ATOM	1480	N	GLU	286	1.096	-23.851	125.710	1.00 37.54	A	N
	ATOM	1481	CA	GLU	286			127.085	1.00 37.97	A	С
40	ATOM	1482	CB	GLU	286	1.526	-22.794	127.884	1.00 39.37	Α	C
	MOTA	1483	CG	GLU	286	2.269	-23.502	128.993	1.00 42.37	Α	C
	ATOM	1484	CD	GLU	286			129.792	1.00 44.10	Α	С
	MOTA	1485		GLU	286			130.402	1.00 45.20	Α	0
	MOTA	1486	OE2	GLU	286	1.612	-25.640	129.803	1.00 46.83	A	0
45	MOTA	1487	С	GLU	286			7 127.167	1.00 36.84	A	С
	ATOM	1488	0	GLU	286			3 128.047	1.00 36.65	Α	0
	MOTA	1489	N	GLU	287	-1.187	-22.37	5 126.251	1.00 37.13	Α	N
	MOTA	1490	CA	GLU	287	-2.541	21.84	8 126.203	1.00 37.20	Α	C
	MOTA	1491	CB	GLU	287			1 125.128	1.00 39.14	Α	C
50	ATOM	1492	CG	GLU	287			5 125.181	1.00 42.57	Α	C
	MOTA	1493		GLU	287			2 124.108	1.00 44.54	A	C
	ATOM	1494		L GLU	287	-2.923	-18.03	1 124.049	1.00 45.67	Α	0
	MOTA	1495		GLU	287			2 123.330	1.00 45.07	A	
	ATOM	1496	C	GLU	287	-3.517	-22.98	7 125.885		A	С
55	MOTA	1497		GLU	287			9 126.514		A	0
	MOTA	1498		MET	288			9 124.907		A	
	ATOM	1499		MET	288	-3.998	3 -24.95	0 124.509	1.00 34.70	Α	
	ATOM	1500		MET	288	-3.384	-25.68	9 123.313	1.00 35.45	A	

-195-

	MOTA	1501	CG	MET	288		-24.841		1.00 36.49	A	C
	MOTA	1502	SD	MET	288		-24.110		1.00 37.77	A	S
	ATOM	1503	CE	MET	288		-22.370		1.00 38.91	A	C
	MOTA	1504	C	MET	288		-25.930		1.00 33.74	A	C
5	MOTA	1505	0	MET	288		-26.379		1.00 33.02	A	0
	MOTA	1506	N	ALA	289	-2.956	-26.260	126.253	1.00 33.19	A	N
	ATOM	1507	CA	ALA	289		-27.195	127.370	1.00 32.47	Α	C
	MOTA	1508	CB	ALA	289			127.826	1.00 31.87	Α	С
	ATOM	1509	C	ALA	289	-3.760	-26.772	128.541	1.00 32.22	A	C
10	ATOM	1510	0	ALA	289	-4.537	-27.575	129.066	1.00 31.24	Α	0
	ATOM	1511	N	LEU	290	-3.634	-25.512	128.948	1.00 32.24	Α	N
	MOTA	1512	CA	LEU	290	-4.420	-24.985	130.055	1.00 32.90	A	C
	MOTA	1513	CB	LEU	290	-4.009	-23.543	130.348	1.00 34.69	Α	C
	ATOM	1514	CG	LEU	290	-2.627	-23.383	130.975	1.00 35.82	A	C
15	ATOM	1515	CD1	LEU	290	-2.309	-21.900	131.153	1.00 36.30	Α	C
	ATOM	1516	CD2	LEU	290	-2.601	-24.111	132.314	1.00 36.19	A	С
	ATOM	1517	С	LEU	290	-5.910	-25.050	129.761	1.00 32.17	A	C
	MOTA	1518	0	LEU	290	-6.707	-25.393	130.628	1.00 32.35	Α	0
	ATOM	1519	N	THR	291	-6.283	-24.713	128.533	1.00 31.75	A	N
20	MOTA	1520	CA	THR	291	-7.680	-24.761	128.124	1.00 31.71	Α	С
	ATOM	1521	CB	THR	291	-7.837	-24.298	126.662	1.00 32.01	A	C
	MOTA	1522	OG1	THR	291	-7.204	-23.022	126.497	1.00 32.68	Α	0
	MOTA	1523	CG2	THR	291	-9.312	-24.179	126.291	1.00 31.69	Α	С
	ATOM	1524	С	THR	291	-8.192	-26.199	128.252	1.00 31.72	A	C
25	MOTA	1525	0	THR	291	-9.289	-26.434	128.760	1.00 31.36	A	0
	MOTA	1526	N	LEU	292	~7.392	-27.159	127.792	1.00 31.96	A	N
	MOTA	1527	CA	LEU	292	-7.772	-28.567	127.864	1.00 32.82	A	C
	ATOM	1528	CB	LEU	292	-6.672	-29.464	127.278	1.00 31.84	Α	С
	MOTA	1529	CG	LEU	292	-7.088	-30.797	126.636	1.00 32.12	Α	С
30	ATOM	1530	CD1	LEU	292	-5.901	-31.753	126.649	1.00 30.55	A	С
	MOTA	1531	CD2	LEU	292	-8.265	-31.413	127.367	1.00 31.13	Α	С
	MOTA	1532	C	LEU	292	-8.005	-28.960	129.318	1.00 33.29	Α	С
	MOTA	1533	0	LEU	292	-9.011	-29.582	129.643	1.00 32.92	Α	0
	MOTA	1534	N	GLN	293	-7.061	-28.606	130.185	1.00 34.69	A	N
35	ATOM	1535	CA	GLN	293	-7.170	-28.920	131.603	1.00 36.33	A	C
	ATOM	1536	CB	GLN	293	-5.973	-28.369	132.368	1.00 37.25	A	С
	ATOM	1537	CG	GLN	293			132.047	1.00 38.64	A	С
	ATOM	1538	CD	GLN	293			132.948	1.00 39.42	A	С
	ATOM	1539	OE1	GLN	293	-3.615	-28.720	134.169	1.00 40.32	Α	0
40	MOTA	1540	NE2	GLN	293	-2.521	-27.966	132.355	1.00 39.89	A	N
	ATOM	1541	С	GLN	293			132.194	1.00 37.50	A	С
	MOTA	1542	0		293			132.852	1.00 37.40	A	0
	MOTA	1543	N	SER	294			131.969	1.00 38.47	Α	N
4.5	MOTA	1544	CA	SER	294			132.480	1.00 39.65	Α	С
45	MOTA	1545	CB	SER	294			131.994	1.00 39.69	Α	С
	MOTA	1546	OG	SER	294			132.355	1.00 40.48	A	0
	MOTA	1547	C	SER	294	-11.092	-27.098	131.996	1.00 40.07	Α	С
	MOTA	1548	0	SER	294			132.770	1.00 40.28	Α	0
	MOTA	1549	N	TYR	295			130.712	1.00 40.29	A	N
50	MOTA	1550	CA	TYR	295			130.129	1.00 41.02	Α	С
	MOTA	1551	CB	TYR	295			128.633	1.00 40.48	Α	С
	MOTA	1552	CG	TYR	295			127.941	1.00 40.03	Α	С
	MOTA	1553		TYR	295			128.033	1.00 39.72	Α	C
	MOTA	1554		TYR	295			127.483	1.00 40.15	A	_
55	ATOM	1555	CD2		295			127.271	1.00 39.70	A	_
	MOTA	1556	CE2		295			126.722	1.00 39.35	A	
	MOTA	1557	CZ	TYR	295			126.834	1.00 40.12	A	
	ATOM	1558	OH	TYR	295	-16.748	-30.399	126.308	1.00 41.32	A	0

-196-

	ATOM	1559		TYR	295	-12.507			1.00 41.79	A	C
	ATOM	1560	0	TYR	295	-13.649			1.00 42.03	A	0
	MOTA	1561	N	ILE	296	-11.455			1.00 42.99	A	N
_	MOTA	1562	CA	ILE	296		-31.532		1.00 44.15	Α	C
5	ATOM	1563	CB	ILE	296		-32.290		1.00 43.14	Α	C
	MOTA	1564	CG2	ILE	296	-10.377	-33.564	132.540	1.00 42.45	A	С
	MOTA	1565	CG1	ILE	296	-9.823	-32.597	130.279	1.00 42.93	Α	С
	ATOM	1566	CD1	ILE	296	-8.468	-33.258	130.163	1.00 41.86	A	С
	ATOM	1567	C	ILE	296		-31.365		1.00 45.76	A	C
10	ATOM	1568	Ō	ILE	296		-32.099		1.00 45.29	A	Ō
	ATOM	1569	N	LYS	297		-30.401	-	1.00 48.10	Α	N
	ATOM	1570	CA	LYS	297		-30.141		1.00 51.07	A	C
	ATOM	1571	CB	LYS	297		-28.985		1.00 51.11	A	c
	ATOM	1572	CG	LYS	297		-29.359		1.00 52.35	A	C
15	ATOM	1573	CD	LYS	297		-28.200		1.00 52.35	A	C
10	ATOM	1574		LYS	297		-28.635				C
			CE						1.00 54.08	A	
	ATOM	1575	NZ	LYS	297		-27.527		1.00 54.48	A	N
	ATOM	1576	C	LYS	297		-29.835		1.00 53.02	A	C
20	MOTA	1577	0	LYS	297			136.328	1.00 53.38	Α	0
20	MOTA	1578	N	GLY	298			134.374	1.00 55.42	A	N
	MOTA	1579	CA	GLY	298			134.397	1.00 58.64	Α	C
	ATOM	1580	C	GLY	298			133.854	1.00 61.18	A	C
	MOTA	1581	0	GLY	298			133.409	1.00 61.26	A	0
	MOTA	1582	N	GLN	299			133.895	1.00 63.92	A	N
25	ATOM	1583	CA	GLN	299			133.405	1.00 66.98	A	C
	ATOM	1584	CB	GLN	299	-15.633	-33.613	133.853	1.00 67.13	A	C
	MOTA	1585	CG	GLN	299	-15.230	-33.657	135.333	1.00 67.29	Α	C
	ATOM	1586	CD	GLN	299	-16.415	-33.750	136.282	1.00 67.70	Α	C
	ATOM	1587	OE1	GLN	299	-17.196	-34.701	136.230	1.00 67.82	Α	0
30	MOTA	1588	NE2	GLN	299			137.161	1.00 67.75	Α	N
	ATOM	1589	C	GLN	299			133.850	1.00 68.93	A	C
	ATOM	1590	Ö	GLN	299			134.831	1.00 69.45	A	ō
	ATOM	1591	N	GLN	300			133.116	1.00 71.11	A	N
	MOTA	1592	CA	GLN	300			133.446	1.00 73.14	A	C
35	ATOM	1593	CB	GLN	300			132.250	1.00 73.51	A	c
	ATOM	1594	CG	GLN	300			131.267	1.00 74.36	A	Č
	ATOM	1595	CD	GLN	300			131.902	1.00 75.03	A	C
	ATOM	1596	OE1		300			132.842	1.00 75.24	A	Ö
	ATOM	1597	NE2		300			131.392	1.00 75.25	A	N
40	ATOM	1598	C	GLN	300			134.661	1.00 73.23	A	C
40	ATOM	1599	0	GLN	300	-20.722		135.700	1.00 74.54	A	Ö
	ATOM	1600	Ŋ	ARG	301			133.700	1.00 74.59		
									1.00 75.65	A	N
	ATOM	1601	CA	ARG	301			135.667		A	C
45	ATOM	1602	CB	ARG	301			135.677	1.00 77.20	A	C
45	MOTA	1603	CG	ARG	301			137.063	1.00 78.13	A	C
	MOTA	1604	CD	ARG	301			137.011	1.00 78.94	A	С
	ATOM	1605	NE	ARG	301			138.344	1.00 79.59	A	N
	MOTA	1606		ARG	301			138.602	1.00 79.96	A	C
	MOTA	1607		ARG	301			139.854	1.00 80.06	A	N
50	MOTA	1608			301			2 137.617	1.00 79.96	A	N
	MOTA	1609		ARG	301			3 135.678	1.00 76.98	Α	С
	MOTA	1610	0	ARG	301			134.788	1.00 76.77	Α	0
	MOTA	1611	N	ARG	302			136.713	1.00 77.23	Α	N
	ATOM	1612		ARG	302	-18.288	3 -39.563	3 136.920	1.00 77.33	Α	С
55	ATOM	1613		ARG	302	-18.689	-40.250	138.232	1.00 77.94	Α	C
	MOTA	1614		ARG	302			139.425	1.00 79.00	Α	
	MOTA	1615		ARG	302			3 140.647	1.00 80.06	A	
	ATOM	1616		ARG	302			5 141.727	1.00 80.81	Α	
											

-197-

	MOTA	1617	_	ARG	302	-20.120			1.00			C
	MOTA	1618		ARG	302	-20.414			1.00		A	N
	MOTA	1619		ARG	302	-20.329			1.00		A	N
_	MOTA	1620	-	ARG	302	-18.432				76.86	A	C
5	MOTA	1621		ARG	302	-19.245			1.00		A	0
	MOTA	1622		PRO	303	-17.641			1.00		Α	N
	MOTA	1623		PRO	303	-17.651			1.00		A	C
	MOTA	1624	CA	PRO	303	-16.638			1.00		A	C
	MOTA	1625	CB	PRO	303	-16.150			1.00		A	C
10	MOTA	1626	CG	PRO	303	-16.298				75.99	A	C
	MOTA	1627	C	PRO	303	-15.502				74.26	A	C
	ATOM	1628	0	PRO	303	-14.879				74.49	A	0
	MOTA	1629	N	ARG	304	-15.251				72.62	A	N
	MOTA	1630	CA	ARG	304	-14.193				70.74	A	C
15	MOTA	1631	CB	ARG	304	-13.927				71.66	A	С
	ATOM	1632	CG	ARG	304	-13.223				72.36	A	С
	MOTA	1633	CD	ARG	304	-14.164				73.27	Α	C
	MOTA	1634	NE	ARG	304	-13.466				73.97	Α	N
	MOTA	1635	CZ	ARG	304	-12.741				74.21	A	C
20	ATOM	1636	NH1	ARG	304	-12.601				74.26	A	N
	MOTA	1637	NH2	ARG	304	-12.154	-45.060	140.473		74.59	A	N
	MOTA	1638	С	ARG	304	-12.909	-40.014	137.716	1.00	68.87	A	C
	MOTA	1639	0	ARG	304		-41.179			68.86	A	0
	MOTA	1640	N	ASP	305		-39.066		1.00	66.37	A	N
25	MOTA	1641	CA	ASP	305	-10.727	-39.378	136.875	1.00	62.94	A	C
	MOTA	1642	CB	ASP	305	-10.978	-40.055	135.525	1.00	63.29	A	С
	MOTA	1643	CG	ASP	305	-9.704	-40.566	134.887	1.00	63.63	A	С
	ATOM	1644	OD1	ASP	305	-8.944	-41.283	135.570	1.00	63.64	Α	0
	MOTA	1645	OD2	ASP	305	-9.465	-40.259	133.701	1.00	64.48	A	0
30	ATOM	1646	C	ASP	305	-9.804	-38.183	136.670	1.00	60.10	A	C
	ATOM	1647	0	ASP	305	-9.951	-37.428	135.704	1.00	59.69	A	0
	MOTA	1648	N	ARG	306	-8.855	-38.005	137.584	1.00	56.47	A	N
	MOTA	1649	CA	ARG	306	-7.896	-36.918	137.437	1.00	52.72	A	С
	MOTA	1650	CB	ARG	306	-7.376	-36.424	138.792	1.00	54.11	Α	C
35	MOTA	1651	CG	ARG	306	-6.551	-35.137	138.659	1.00	55.62	Α	C
	ATOM	1652	CD	ARG	306	-5.264	-35.152	139.480	1.00	57.19	A	С
	MOTA	1653	NE	ARG	306	-5.384	-34.423	140.743	1.00	58.88	Α	N
	ATOM	1654	CZ	ARG	306	-4.358	-34.121	141.537	1.00	59.27	Α	C
	ATOM	1655	NH1	ARG	306	-3.125	-34.487	141.204	1.00	59.61	A	N
40	ATOM	1656	NH2	ARG	306	-4.561	-33.443	142.662	1.00	59.29	Α	N
	MOTA	1657	С	ARG	306			136.612		49.02	A	С
	MOTA	1658	0	ARG	306			136.448		49.06	Α	0
	MOTA	1659	N	PHE	307			136.101		44.87	Α	N
	ATOM	1660	CA	PHE	307	-5.828	-39.299	135.288		40.64	A	C
45	ATOM	1661	CB	PHE	307			135.477		39.73	Α	C
	MOTA	1662	CG	PHE	307			136.880		39.02	A	C
	MOTA	1663	CD1	PHE	307			137.349		38.54	Α	С
	MOTA	1664	CD2	PHE	307	-6.644	-41.615	137.738	1.00	38.66	Α	C
	ATOM	1665	CE1	. PHE	307			138.650	1.00	38.12	A	C
50	MOTA	1666	CE2	PHE	307			139.044		39.04	A	C
	ATOM	1667	CZ	PHE	307	-5.072	-42.112	139.499		38.17	A	C
	ATOM	1668	С	PHE	307	-5.976	-38.982	133.796		38.25	Α	С
	MOTA	1669	0	PHE	307	-5.036	-39.160	133.026	1.00	36.74	Α	0
	ATOM	1670		LEU	308			133.391		35.76	Α	N
55	ATOM	1671	CA	LEU	308			131.984		33.41	A	С
	ATOM	1672	CB	LEU	308	-8.819	-37.672	131.792		33.07	A	С
	MOTA	1673		LEU	308	-9.360	-37.618	130.351		33.17	A	
	MOTA	1674		LEU	308		-36.444	129.613	1.00	34.19	A	
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WO 2005/019239 PCT/US2004/023092

-198-

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	MOTA	1675	CD2		308	-9.036 -38.913 129.623 1.00 31.34 A C	
	ATOM	1676		LEU	308	-6.389 -37.268 131.337 1.00 31.73 A C	
	ATOM	1677		LEU	308	-5.809 -37.601 130.306 1.00 30.35 A O	
E	ATOM	1678		TYR	309	-6.176 -36.097 131.928 1.00 29.96 A N	
5	MOTA	1679		TYR	309	-5.236 -35.149 131.346 1.00 28.55 A C	
	MOTA	1680		TYR	309	-5.156 -33.865 132.171 1.00 28.94 A C	
	MOTA	1681		TYR	309	-4.250 -32.828 131.543 1.00 29.27 A C	
	MOTA	1682		TYR	309	-4.567 -32.250 130.312 1.00 29.24 A C	
40	MOTA	1683		TYR	309	-3.719 -31.315 129.715 1.00 29.07 A C	
10	MOTA	1684		TYR	309	-3.061 -32.443 132.162 1.00 29.31 A C	
	MOTA	1685	_	TYR	309	-2.209 -31.511 131.573 1.00 29.09 A C	
	MOTA	1686	CZ	TYR	309	-2.544 -30.955 130.353 1.00 28.97 A C	
	MOTA	1687	ОН	TYR	309	-1.697 -30.049 129.766 1.00 29.80 A O	
4-5	MOTA	1688	С	TYR	309	-3.842 -35.738 131.198 1.00 27.07 A C	
15	MOTA	1689	0	TYR	309	-3.204 -35.558 130.169 1.00 26.88 A O	
	MOTA	1690	N	ALA	310	-3.368 -36.436 132.225 1.00 25.89 A N	
	MOTA	1691	CA	ALA	310	-2.049 -37.051 132.169 1.00 25.16 A C	
	ATOM	1692	CB	ALA	310	-1.702 -37.690 133.512 1.00 24.32 A C	
	MOTA	1693	C	ALA	310	-1.997 -38.096 131.046 1.00 24.96 A C	
20	MOTA	1694	0	ALA	310	-1.023 -38.142 130.291 1.00 24.12 A O	
	ATOM	1695	N	LYS	311	-3.036 -38.930 130.940 1.00 23.97 A N	
	MOTA	1696	CA	LYS	311	-3.097 -39.938 129.881 1.00 24.13 A C	
	MOTA	1697	CB	LYS	311	-4.391 -40.752 129.960 1.00 25.00 A C	
	MOTA	1698	CG	LYS	311	-4.473 -41.760 131.105 1.00 27.78 A C	
25	MOTA	1699	CD	LYS	311	-5.831 -42.472 131.058 1.00 29.79 A C	
	MOTA	1700	CE	LYS	311	-6.089 -43.328 132.285 1.00 31.20 A C	
	MOTA	1701	NZ	LYS	311	-7.505 -43.836 132.302 1.00 33.50 A N	
	MOTA	1702	С	LYS	311	-3.031 -39.268 128.508 1.00 23.70 A C	
	MOTA	1703	0	LYS	311	-2.430 -39.806 127.583 1.00 23.05 A O	
30	ATOM	1704	N	LEU	312	-3.651 -38.098 128.378 1.00 22.94 A N	
	ATOM	1705	CA	LEU	312	-3.643 -37.380 127.113 1.00 23.55 A C	
	ATOM	1706	CB	LEU	312	-4.656 -36.230 127.143 1.00 24.36 A C	
	ATOM	1707	CG	LEU	312	-6.128 -36.661 127.073 1.00 25.69 A C	
	MOTA	1708	CD1	LEU	312	-7.026 -35.447 126.879 1.00 24.81 A C	
35	ATOM	1709	CD2	LEU	312	-6.312 -37.629 125.910 1.00 26.15 A C	
	ATOM	1710	С	LEU	312	-2.248 -36.860 126.748 1.00 23.28 A C	
	MOTA	1711	0	LEU	312	-1.859 -36.888 125.580 1.00 22.28 A O)
	MOTA	1712	N	LEU	313	-1.498 -36.374 127.733 1.00 22.16 A N	ľ
	MOTA	1713	CA	LEU	313	-0.145 -35.905 127.460 1.00 22.07 A C	
40	MOTA	1714	CB	LEU	313	0.454 -35.225 128.694 1.00 21.00 A C	
	MOTA	1715	CG	LEU	313	-0.202 -33.891 129.064 1.00 21.22 A C	
	MOTA	1716	CD1	LEU	313	0.485 -33.316 130.284 1.00 20.26 A C	
	MOTA	1717	CD2	LEU	313	-0.115 -32.920 127.886 1.00 18.10 A C	
	ATOM	1718	С	LEU	313	0.681 -37.131 127.059 1.00 22.48 A C	•
45	MOTA	1719	0	LEU	313	1.512 -37.068 126.152 1.00 22.20 A O)
	ATOM	1720	N	GLY	314	0.434 -38.251 127.733 1.00 22.89 A N	
	ATOM	1721	CA	GLY	314	1.131 -39.479 127.402 1.00 23.30 A C	
	ATOM	1722	C	GLY	314	0.860 -39.842 125.949 1.00 23.94 A C	
	MOTA	1723	0	GLY	314	1.782 -40.168 125.200 1.00 24.54 A O)
50	MOTA	1724	N	LEU	315	-0.410 -39.779 125.549 1.00 23.59 A N	
	MOTA	1725	CA	LEU	315	-0.807 -40.092 124.182 1.00 22.89 A C	
	MOTA	1726	CB	LEU	315	-2.336 -40.134 124.070 1.00 23.44 A C	
	MOTA	1727	CG	LEU	315	-2.961 -41.398 124.681 1.00 23.97 A C	;
<u></u>	MOTA	1728	CD1	LEU	315	-4.465 -41.270 124.742 1.00 23.92 A C	:
55	MOTA	1729	CD2	LEU	315	-2.566 -42.613 123.854 1.00 23.72 A C	;
	MOTA	1730	C	LEU	315	-0.221 -39.115 123.167 1.00 22.47 A C	;
	MOTA	1731		LEU	315	0.094 -39.505 122.044 1.00 22.11 A C	
	ATOM	1732		LEU	316	-0.072 -37.849 123.544 1.00 22.35 A N	1

-199-

	ATOM	1733	CA	LEU	316	0.524	-36.882	122.626	1.00 22.93	A	C
	ATOM	1734	CB	LEU	316	0.454	-35.465	123.194	1.00 23.82	A	C
	MOTA	1735	CG	LEU	316	-0.934	-34.817	123.164	1.00 25.69	A	C
	ATOM	1736	CD1	LEU	316	-0.879	-33.440	123.802	1.00 25.97	A	C
5	MOTA	1737	CD2	LEU	316	-1.418	-34.720	121.722	1.00 26.87	A	C
	ATOM	1738	С	LEU	316	1.977	-37.273	122.401	1.00 23.05	Α	C
	ATOM	1739	0	LEU	316			121.290	1.00 23.13	A	0
	MOTA	1740	N	ALA	317		-37.741		1.00 22.68	A	N
	MOTA	1741	CA	ALA	317		-38.169		1.00 23.73	A	C
10	ATOM	1742	CB	ALA	317		-38.439		1.00 23.13	A	C
	MOTA	1743	С	ALA	317		-39.426		1.00 23.75	A	Ċ
	ATOM	1744	ō	ALA	317		-39.567		1.00 22.15	A	ō
	MOTA	1745	N	GLU	318		-40.334		1.00 24.36	A	N
	MOTA	1746	CA	GLU	318		-41.562		1.00 26.08	A	C
15	MOTA	1747	СВ	GLU	318		-42.543		1.00 28.21	A	Č
	ATOM	1748	CG	GLU	318		-43.831		1.00 32.51	A	Ċ
	ATOM	1749	CD	GLU	318		-45.004		1.00 35.59	A	C
	ATOM	1750	OE1		318		-45.114		1.00 36.82	A	ō
	ATOM	1751		GLU	318			122.796	1.00 38.53	A	ŏ
20	ATOM	1752	C	GLU	318			120.391	1.00 25.72	A	Č
	ATOM	1753	ŏ	GLU	318			119.557	1.00 24.88	A	ŏ
	ATOM	1754	N	LEU	319			120.068	1.00 25.55	A	N
	ATOM	1755	CA	LEU	319			118.684	1.00 25.73	A	C
	ATOM	1756	CB	LEU	319			118.652	1.00 24.34	A	Č
25	ATOM	1757	CG	LEU	319			117.311	1.00 24.57	A	C
	ATOM	1758		LEU	319			116.426	1.00 21.78	A	Č
	ATOM	1759		LEU	319			117.576	1.00 23.45	A	C
	ATOM	1760	C	LEU	319			118.103	1.00 26.16	A	Č
	ATOM	1761	ŏ	LEU	319			116.907	1.00 26.27	A	Ö
30	ATOM	1762	N	ARG	320			118.969	1.00 26.63	Α	N
	ATOM	1763	CA	ARG	320			118.587	1.00 27.47	A	C
	ATOM	1764	СВ	ARG	320			119.786	1.00 29.62	A	C
	ATOM	1765	CG	ARG	320			119.463	1.00 32.70	A	Č
	ATOM	1766	CD	ARG	320			118.741	1.00 35.19	A	C
35	MOTA	1767	NE	ARG	320			118.307	1.00 36.76	A	N
•	ATOM	1768	CZ	ARG	320			118.624	1.00 37.53	A	C
	ATOM	1769	NH1		320			119.389	1.00 37.83	A	N
	ATOM	1770	NH2		320			118.166	1.00 37.03	A	N
	ATOM	1771	C	ARG	320			118.169	1.00 26.95	A	C
40	ATOM	1772	Ö	ARG	320	6.849			1.00 27.09	A	o
. •	ATOM	1773	N	SER	321			118.898	1.00 25.51	A	N
	ATOM	1774	CA	SER	321			118.603		A	
	ATOM	1775	СВ	SER	321			119.661	1.00 24.40	A	C
	ATOM	1776	OG	SER	321			120.843	1.00 26.98	A	Ö
45	ATOM	1777	C	SER	321			117.261	1.00 24.22	A	Č
	ATOM	1778	ŏ	SER	321			116.450	1.00 23.84	A	Ö
	ATOM	1779	N	ILE	322			117.051	1.00 23.23	A	N
	ATOM	1780	CA	ILE	322			115.810	1.00 23.56	A	C
	ATOM	1781	СВ	ILE	322			115.876	1.00 23.28	A	C
50	ATOM	1782	CG2		322			114.484	1.00 22.26	A	C
	ATOM	1783		ILE	322			116.855	1.00 22.75	A	C
	ATOM	1784		ILE	322			117.140	1.00 21.11	A	C
	ATOM	1785	C	ILE	322			114.639	1.00 21.11	A	C
	ATOM	1786	Ö	ILE	322			113.590	1.00 24.10	A	0
55	ATOM	1787	N	ASN				114.826	1.00 24.50	A	
J J	ATOM	1788	CA	ASN	323			114.828		A	N
	ATOM	1789	CB	ASN	323			113.767		A	C
	ATOM	1790	CG	ASN				113.244			C
	ATOM	1/50	CG	V91A	343	3.309	-31.41	113.244	1.00 30.34	A	С

-200-

	ATOM	1791	OD1	ASN	323	6.870	-37.489	112.509	1.00 33.18	A	0
	ATOM	1792	ND2	ASN	323		-36.148		1.00 31.75	A	N
	ATOM	1793	С	ASN	323	6.953	-40.100	113.408	1.00 25.95	A	С
	ATOM	1794	0	ASN	323	7.265	-40.282	112.236	1.00 25.34	A	0
5	ATOM	1795	N	GLU	324		-40.232		1.00 26.65	A	N
	MOTA	1796	CA	GLU	324	9.208	-40.597	114.173	1.00 27.58	A	C
	MOTA	1797	СВ	GLU	324			115.482	1.00 30.21	A	C
	MOTA	1798	CG	GLU	324	9.920	-39.180		1.00 34.60	A	C
	MOTA	1799	CD	GLU	324	10.646	-39.163		1.00 37.84	A	C
10	ATOM	1800	OE1		324		-40.138		1.00 39.66	A	Ō
	ATOM	1801	OE2		324		-38.173		1.00 39.51	Α	Ŏ
	ATOM	1802	C	GLU	324		-41.988		1.00 26.74	A	C
	MOTA	1803	0	GLU	324		-42.221		1.00 26.19	A	ō
	ATOM	1804	N	ALA	325		-42.914		1.00 25.09	A	N
15	MOTA	1805	CA	ALA	325		-44.258		1.00 25.00	A	c
. •	ATOM	1806	СВ	ALA	325		-45.209		1.00 24.73	A	c
	MOTA	1807	c	ALA	325		-44.238		1.00 24.89	A	Č
	ATOM	1808	ŏ	ALA	325		-45.073		1.00 25.47	A	ŏ
	ATOM	1809	N	TYR	326		-43.297		1.00 23.96	A	N
20	MOTA	1810	CA	TYR	326		-43.145		1.00 23.70	A	C
	ATOM	1811	CB	TYR	326		-41.988		1.00 23.70	A	C
	ATOM	1812	CG	TYR	326		-42.402		1.00 22.03		C
	ATOM	1813		TYR	326		-43.180		1.00 21.43	A	c
	ATOM	1814	CE1	TYR	326		-43.541		1.00 20.69	A	C
25	MOTA	1815	CD2		326			110.897	1.00 19.55	A	C
20	ATOM	1816	CE2	TYR	326			110.837	1.00 21.09	A	
	MOTA	1817	CZ	TYR	326			109.791	1.00 20.21	A	C
	MOTA	1818	OH	TYR	326			109.791	1.00 20.21	A	o
	MOTA	1819	C	TYR	326			109.749	1.00 19.33	A	
30	ATOM	1820	0	TYR	326			109.280	1.00 23.33	A	C
00	ATOM	1821	N	GLY	327			109.802	1.00 25.27	A	0
	ATOM	1822	CA	GLY	327		-41.563			A	И
	ATOM							109.110	1.00 26.47	A	C
	ATOM	1823 1824	C O	GLY GLY	327 327			108.912	1.00 27.58	A	C
35	ATOM	1825			327			107.848	1.00 27.44	A	0
00	ATOM	1826	N	TYR	328				1.00 29.10	A	N
			CA CB	TYR				109.838	1.00 30.30	A	C
	MOTA	1827		TYR	328			111.182	1.00 31.95	A	C
	ATOM	1828	CG CD1	TYR	328		-46.839 -46.930	111.127	1.00 33.79	A	C
40	MOTA	1829	CD1		328				1.00 35.24	A	C
40	MOTA	1830	CE1		328			111.242	1.00 36.06	A	C
	ATOM	1831	CD2		328			110.778 110.652	1.00 34.19	A	C
	ATOM	1832		TYR	328				1.00 35.21	A	
	ATOM	1833	CZ	TYR	328			110.884	1.00 36.45	A	C
45	ATOM	1834	ОН	TYR	328			110.736	1.00 37.83	A	0
73	ATOM	1835	C	TYR	328			108.758	1.00 30.82	A	С
	ATOM	1836	0	TYR	328			107.966	1.00 30.88	A	0
	ATOM	1837	N	GLN	329			108.737	1.00 31.03	A	N
	ATOM	1838	CA	GLN	329			107.759	1.00 31.18	A	C
50	MOTA	1839	CB	GLN	329			108.011	1.00 29.87	Α	C
50	ATOM	1840	CG	GLN	329			109.377	1.00 30.38	A	С
	MOTA	1841	CD	GLN	329			109.523	1.00 31.26	Α	C
	ATOM	1842		GLN	329			110.338	1.00 30.58	A	0
	ATOM	1843		GLN	329			108.729	1.00 30.24	A	N
EE	MOTA	1844	C	GLN	329			106.338	1.00 31.84	A	C
55	ATOM	1845	0	GLN	329			105.457	1.00 31.67	Α	0
	ATOM	1846	N	ILE	330			106.118	1.00 32.78	Α	N.
	MOTA	1847		ILE	330			104.800	1.00 34.51	Α	C
	MOTA	1848	CB	ILE	330	9.423	-42.833	104.798	1.00 34.57	Α	C

-201-

	MOTA	1849	CG2		330		-42.113		1.00 34.87	A	C
	MOTA	1850	CG1		330		-42.697		1.00 34.64	A	С
	MOTA	1851	CD1		330		-41.267	104.779	1.00 35.62	A	C
_	MOTA	1852	C	ILE	330	11.231	-44.519	104.300	1.00 35.74	A	C
5	MOTA	1853	0	ILE	330	11.467	-44.599	103.094	1.00 34.91	A	0
	MOTA	1854	N	GLN	331	12.179	-44.604	105.228	1.00 37.46	Α	N
	MOTA	1855	CA	GLN	331	13.586	-44.776	104.882	1.00 39.69	A	С
	ATOM	1856	СВ	GLN	331		-44.235		1.00 42.13	A	С
	ATOM	1857	CG	GLN	331	_		106.134	1.00 44.67	A	C
10	MOTA	1858	CD	GLN	331		-42.325	107.428	1.00 47.11	A	Ċ
. •	ATOM	1859	OE1		331		-42.870		1.00 48.26	A	ō
	MOTA	1860		GLN	331		-41.362		1.00 48.66	A	N
	MOTA	1861	C	GLN	331		-46.211		1.00 39.80	A	C
		1862			331		-46.463		1.00 39.80		0
16	MOTA		0	GLN						A	
15	MOTA	1863	N	HIS	332		-47.155		1.00 39.86	A	N
	MOTA	1864	CA	HIS	332		-48.546		1.00 40.67	Α	C
	ATOM	1865	CB	HIS	332		-49.161		1.00 42.81	A	C
	MOTA	1866	CG	HIS	332		-48.524		1.00 46.28	A	C
	MOTA	1867		HIS	332			108.086	1.00 47.01	Α	C
20	ATOM	1868		HIS	332			107.275	1.00 47.57	A	N
	ATOM	1869		HIS	332	17.256	-48.181	107.961	1.00 47.73	Α	C
	MOTA	1870	NE2	HIS	332	16.518	-47.208	108.461	1.00 48.10	A	N
	MOTA	1871	C	HIS	332	12.928	-49.422	104.337	1.00 39.76	A	C
	ATOM	1872	0	HIS	332	13.241	-50.587	104.082	1.00 39.61	A	0
25	MOTA	1873	N	ILE	333	11.810	-48.871	103.882	1.00 38.23	A	N
	MOTA	1874	CA	ILE	333	10.900	-49.647	103.055	1.00 37.05	Α	C
	ATOM	1875	СВ	ILE	333	9.567	-49.887	103.779	1.00 36.60	A	C
	ATOM	1876	CG2		333			102.878	1.00 36.04	A	C
	ATOM	1877		ILE	333			105.066	1.00 37.04	A	Č
30	ATOM	1878	CD1		333			105.963	1.00 36.04	A	Ċ
•	ATOM	1879	C	ILE	333			101.713	1.00 36.44	A	Č
	ATOM	1880	Ö	ILE	333			101.599	1.00 36.09	A	ŏ
	ATOM	1881	N	GLN	334			100.707	1.00 35.60	A	N
	MOTA	1882	CA	GLN	334		-48.909		1.00 35.00	A	C
35					334		-49.788		1.00 37.05		C
33	ATOM	1883	CB	GLN						A	
	MOTA	1884	CG	GLN	334		-49.113		1.00 40.94	A	C
	ATOM	1885	CD	GLN	334		-48.947		1.00 43.49	A	C
	ATOM	1886	OE1		334		-48.031		1.00 45.60	A	0
40	ATOM	1887	NE2		334		-49.846		1.00 44.60	A	N
40	ATOM	1888	С	GLN	334		-48.925		1.00 33.48	A	C
	MOTA	1889	0	GLN	334		-49.929		1.00 32.53	Α	0
	MOTA	1890	N	GLY	335		-47.801		1.00 32.61	A	N
	MOTA	1891	CA	GLY	335		-47.724		1.00 31.27	Α	С
	MOTA	1892	C	GLY	335		-47.059		1.00 30.52	A	С
45	ATOM	1893	0	GLY	335		-46.519		1.00 29.45	A	0
	MOTA	1894	N	LEU	336			100.122	1.00 30.35	A	N
	MOTA	1895	CA	LEU	336	6.371	-46.474	101.073	1.00 30.47	Α	C
	ATOM	1896	CB	LEU	336	6.837	-46.683	102.515	1.00 30.60	Α	С
	ATOM	1897	CG	LEU	336	6.505	-47.973	103.265	1.00 31.59	A	C
50	MOTA	1898	CD1	LEU	336	6.881	-47.777	7 104.731	1.00 32.05	Α	C
	MOTA	1899		LEU	336	5.027	-48.308	3 103.153	1.00 31.01	Α	С
	MOTA	1900		LEU	336			100.845		Α	Č
	ATOM	1901	ō	LEU	336			7 100.891	1.00 29.66	A	
	MOTA	1902		SER	337			100.603		A	
55	ATOM	1903		SER	337		-42.829			A	C
55	MOTA	1903		SER	337			7 100.333		A	
	ATOM	1904		SER	337		-42.77			A	
										A	
	MOTA	1906	С	SER	337	0.286	-42.419	99.263	1.00 32.68	A	С

-202-

													_
	MOTA	1907		SER	337	5.792			99.246	1.00			0
	MOTA	1908		ALA	338	6.030			98.324	1.00	-		N
	MOTA	1909	-	ALA	338	5.133			97.218	1.00			C
Ę.	MOTA	1910		ALA	338	5.072			96.257	1.00			C
5	MOTA	1911	_	ALA	338	3.723	-42.		97.711	1.00		A	C
	MOTA	1912	_	ALA	338	2.979			97.032	1.00		A	0
	MOTA	1913		MET	339	3.348			98.879	1.00		A	N
	MOTA	1914		MET	339	2.024			99.422	1.00		A	C
40	MOTA	1915		MET	339	1.604			100.400	1.00		A	C
10	MOTA	1916	CG	MET	339		-45.		99.701		29.56	A	C
	MOTA	1917	SD	MET	339				100.838		26.76	A	S
	MOTA	1918	CE	MET	339				101.313		25.89	A	C
	MOTA	1919	С	MET	339				100.086		38.11	A	C
4=	MOTA	1920	0	MET	339				100.475		38.51	A	0
15	MOTA	1921	N	MET	340				100.217		41.19	A	N
	MOTA	1922	CA	MET	340				100.792		45.17	A	C
	ATOM	1923	CB	MET	340				102.108		45.06	A	C
	MOTA	1924	CG	MET	340				102.892		45.91	A	C
	MOTA	1925	SD	MET	340				103.173		46.05	A	S
20	MOTA	1926	CE	MET	340				101.643		45.26	Α	C
	MOTA	1927	C	MET	340	3.848			99.793		48.30	A	C
	MOTA	1928	0	MET	340				100.023		48.09	A	0
	MOTA	1929	N	PRO	341	3.180			98.662		51.89	A	N
05	MOTA	1930	CD	PRO	341	1.818			98.307		52.61	A	C
25	MOTA	1931	CA	PRO	341	3.725			97.616		55.17	A	C
	MOTA	1932	CB	PRO	341	2.552			96.649		54.46	A	C
	MOTA	1933	CG	PRO	341	1.812			96.810		53.80	Α	C
	MOTA	1934	С	PRO	341	4.201					58.43	A	С
00	MOTA	1935	0	PRO	341	5.399					58.94	A	0
30	MOTA	1936	N	LEU	342	3.244				-	61.89	A	N
	MOTA	1937	CA	LEU	342	3.538					65.33	A	C
	MOTA	1938	CB	LEU	342	2.297					65.46	A	C
	MOTA	1939	CG	LEU	342	1.863					65.98	Α	С
0.5	MOTA	1940	_	LEU	342	1.636					66.50	A	C
35	MOTA	1941	_	LEU	342	0.586					66.63	A	C
	MOTA	1942	С	LEU	342	3.956					67.54	A	C
	MOTA	1943	0	LEU	342	3.808					67.71	A	0
	MOTA	1944	N	LEU	343				101.110		70.31	A	N
40	MOTA	1945	CA	LEU	343	4.909					73.10	A	C
40	MOTA	1946	CB	LEU	343				103.401		73.06	A A	C
	MOTA	1947	CG	LEU	343				104.783				
	MOTA	1948		LEU	343				105.615		73.35	A	
	MOTA	1949		LEU	343				104.613		73.19	A	C
AE	MOTA	1950		LEU	343				102.919		75.75	A A	C
45	MOTA	1951		LEU	343						77.19	A	0
	MOTA	1952		GLN	344				102.908				И
	MOTA	1953		GLN	344				103.303		79.02	A A	C
	MOTA	1954		GLN	344				102.552		79.26 79.55	A	C
EΩ	ATOM	1955		GLN	344				5 101.062 5 100.495		79.33	A	C
50	MOTA	1956		GLN	344								
	ATOM	1957		1 GLN	344	8.35					80.00 79.76	A A	O
	ATOM	1958		2 GLN	344				101.366		80.26		N
	ATOM	1959		GLN	344				103.034		80.26		
EF	ATOM	1960		GLN	344				102.587				
55	MOTA	1961		GLU	345				5 103.314 5 103 003		81.48		
	MOTA	1962			345				5 103.093		82.57 83.18		
	MOTA	1963			345				5 104.182 2 105.598		9 83.18 9 84.08		
	MOTA	1964	1 CG	GLU	345	12.22	<i>,</i> –3	J. 5U.	2 TOD.DAR	1.00	. 04.00		

-203-

	ATOM	1965	CD	GLU	345	13.093 -36.500 106.634 1.00 84.62 A	A C
	ATOM	1966	OE1		345		A 0
	ATOM	1967	OE2		345		A 0
	ATOM	1968		GLU	345		A C
5	ATOM	1969		GLU	345		A O
•	ATOM	1970		GLU	345		A O
	TER	1971	•	GLU	345		A.
	ATOM	1972	СВ	PRO	103		ВС
	ATOM	1973	CG	PRO	103		ВС
10	ATOM	1974	C	PRO	103		ВС
••	ATOM	1975	ŏ	PRO	103		во
	ATOM	1976	N	PRO	103		BN
	ATOM	1977	CD	PRO	103		ВС
	ATOM	1978	CA	PRO	103		ВС
15	ATOM	1979	N	VAL	104		BN
. •	ATOM	1980	CA	VAL	104		ВС
	ATOM	1981	СВ	VAL	104		ВС
	ATOM	1982		VAL	104		ВС
	ATOM	1983		VAL	104		вс
20	ATOM	1984	C	VAL	104		вс
	ATOM	1985	Ō	VAL	104		во
	ATOM	1986	N	GLN	105		B N
	ATOM	1987	CA	GLN	105		в с
	ATOM	1988	СВ	GLN	105		вс
25	ATOM	1989	CG	GLN	105		ВС
	ATOM	1990	CD	GLN	105		вс
	ATOM .	1991	OE1	GLN	105		во
	ATOM	1992	NE2	GLN	105		B N
	ATOM	1993	C	GLN	105		вс
30	ATOM	1994	0	GLN	105		во
	ATOM	1995	N	LEU	106	13.067 -92.618 134.273 1.00 72.54	B N
	MOTA	1996	CA	LEU	106	13.747 -93.115 133.070 1.00 70.12	вс
	MOTA	1997	CB	LEU	106	15.259 -92.860 133.160 1.00 70.25	в с
	MOTA	1998	CG	LEU	106	15.813 -91.432 133.205 1.00 70.18	вс
35	ATOM	1999	CD1	LEU	106	15.723 -90.881 134.616 1.00 70.47	в с
	MOTA	2000	CD2	LEU	106	17.267 -91.442 132.752 1.00 69.72	в с
	ATOM	2001	C	LEU	106	13.521 -94.596 132.761 1.00 68.42	ВС
	MOTA	2002	0	LEU	106	14.449 -95.402 132.853 1.00 68.15	в о
	MOTA	2003	N	SER	107	12.295 -94.949 132.382 1.00 66.23	B N
40	ATOM	2004	CA	SER	107	11.955 -96.333 132.064 1.00 63.76	в с
	MOTA	2005	CB	SER	107	10.469 -96.441 131.721 1.00 63.69	в с
	MOTA	2006	OG	SER	107	10.152 -97.713 131.185 1.00 63.42	в о
	MOTA	2007	С	SER	107	12.782 -96.865 130.904 1.00 62.28	в с
	ATOM	2008	0	SER	107	13.328 -96.097 130.117 1.00 62.13	в о
45	MOTA	2009		LYS	108	12.878 -98.187 130.806 1.00 60.42	B N
	MOTA	2010		LYS	108	13.633 -98.817 129.733 1.00 58.34	ВС
	ATOM	2011		LYS	108	13.706-100.328 129.957 1.00 59.09	в с
	MOTA	2012		LYS	108	14.716-101.043 129.078 1.00 59.82	в с
	MOTA	2013		LYS	108	16.139-100.630 129.430 1.00 61.01	в с
50	MOTA	2014		LYS	108	17.167-101.382 128.589 1.00 61.73	ВС
	ATOM	2015		LYS	108	18.572-101.025 128.958 1.00 62.47	ВИ
	MOTA	2016		LYS	108	12.929 -98.524 128.415 1.00 56.63	ВС
	MOTA	2017		LYS	108	13.524 -97.970 127.491 1.00 56.15	во
	ATOM	2018		GLU	109	11.654 -98.895 128.342 1.00 54.51	B N
55	MOTA	2019		GLU	109	10.846 -98.673 127.148 1.00 52.68	ВС
	MOTA	2020		GLU	109	9.464 -99.323 127.297 1.00 53.23	ВС
	MOTA	2021		GLU	109	9.004 -99.560 128.730 1.00 54.59	ВС
	MOTA	2022	CD	GLU	109	9.624-100.809 129.340 1.00 55.04	в с

-204-

	3.000	2022	0.01	OT 11	100	0 370	101 014	100 000	4 00 55 00	_	_
	ATOM	2023	OE1		109			128.809	1.00 55.28	В	0
	ATOM	2024		GLU	109			130.343	1.00 55.07	В	0
	ATOM	2025	C	GLU	109			126.819	1.00 50.98	В	C
5	MOTA	2026	0	GLU	109			125.662	1.00 50.38	В	0
)	ATOM	2027	N	GLN	110			127.832	1.00 49.17	В	N
	MOTA	2028	CA	GLN	110			127.607	1.00 47.33	В	C
	MOTA	2029	CB	GLN	110			128.926	1.00 47.12	В	C
	MOTA	2030	CG	GLN	110			129.606	1.00 47.16	В	С
	MOTA	2031	CD	GLN	110	8.874	-93.656	130.870	1.00 47.26	В	С
10	MOTA	2032	OE1	GLN	110	9.767	-93.545	131.711	1.00 46.64	В	0
	MOTA	2033	NE2	GLN	110	7.682	-93.086	131.014	1.00 47.72	В	N
	MOTA	2034	С	GLN	110	11.896	-94.386	126.921	1.00 46.46	В	C
•	ATOM	2035	0	GLN	110	11.815	-93.558	126.018	1.00 45.75	В	0
	ATOM	2036	N	GLU	111	13.061	-94.871	127.343	1.00 45.39	В	N
15	ATOM	2037	CA	GLU	111			126.714	1.00 44.94	В	C
	ATOM	2038	CB	GLU	111			127.436	1.00 46.33	В	Č
	ATOM	2039	CG	GLU	111			128.924	1.00 48.97	В	Č
	ATOM	2040	CD	GLU	111			129.479	1.00 50.99	В	Č
	ATOM	2041		GLU	111			129.335	1.00 51.59	В	ŏ
20	ATOM	2042		GLU	111			130.049	1.00 51.77	В	ŏ
	MOTA	2043	C	GLU	111			125.262	1.00 43.27	В	c
	ATOM	2044	Ö	GLU	111			124.362	1.00 42.84	В	o
	ATOM	2045	N	GLU	112			124.302	1.00 42.84	В	N
	ATOM	2045	CA	GLU	112				1.00 41.39		
25	ATOM	2040	CB	GLU	112			123.724 123.833	1.00 39.73	В	C
25	ATOM	2047	CG	GLU	112			123.633	1.00 40.89	В	
			CD							В	C
	MOTA MOTA	2049		GLU	112 112			121.624	1.00 44.55	В	C
	ATOM	2050 2051	OE1	GLU GLU	112			122.139 120.419	1.00 45.11 1.00 46.10	В	0
30	ATOM	2052	C	GLU	112			120.419		В	0
50	ATOM	2052	0	GLU	112			121.666	1.00 38.09	В	
	ATOM	2054		LEU	113			121.666	1.00 37.26	В	0
		2055	N	LEU	113				1.00 35.31	В	N
	ATOM	2056	CA CB	LEU	113			122.729	1.00 33.09	В	C
35	ATOM							123.637	1.00 32.27	В	C
33	ATOM	2057	CG	LEU	113			123.101	1.00 32.57	В	C
	ATOM	2058		LEU	113			121.731	1.00 31.91	В	C
	MOTA	2059		LEU	113			124.080	1.00 31.00	В	C
	ATOM	2060	C	LEU	113			122.294	1.00 31.56	В	C
40	MOTA	2061	0	LEU	113			121.138	1.00 30.78	В	0
40	MOTA	2062	N	ILE	114			123.227	1.00 30.06	В	N
	MOTA	2063	CA	ILE	114			122.949	1.00 29.43	В	C
	MOTA	2064	СВ	ILE	114		-90.822		1.00 28.14	В	C
	MOTA	2065		ILE	114			123.870	1.00 27.33	В	C
4-	MOTA	2066		ILE	114			125.228	1.00 27.74	В	С
45	ATOM	2067		ILE	114			3 126.541	1.00 26.41	В	С
	MOTA	2068	С	ILE	114			121.836	1.00 29.65	В	C
	ATOM	2069	0	ILE	114			120.872	1.00 28.66	В	0
	MOTA	2070	N	ARG	115	14.672	-92.571	l 121.961	1.00 30.65	В	N
	ATOM	2071	CA	ARG	115	15.686	-92.821	L 120.947	1.00 32.09	В	С
50	MOTA	2072	CB	ARG	115	16.540	-94.037	7 121.319	1.00 34.79	В	С
	ATOM	2073	CG	ARG	115			7 120.729	1.00 39.78	В	С
	MOTA	2074	CD	ARG	115	18.821	-95.166	5 121.077	1.00 43.64	В	C
	MOTA	2075	NE	ARG	115			1 120.292	1.00 47.79	В	N
	MOTA	2076	CZ	ARG	115			3 120.612	1.00 49.59	В	C
55	ATOM	2077		ARG	115			4 121.713	1.00 51.59	В	N
	MOTA	2078		ARG	115			1 119.832			N
	ATOM	2079	С	ARG	115			6 119.562			C
	ATOM	2080	Ö	ARG	115			6 118.571			

-205-

	MOTA	2081	N	THR	116		-93.734		1.00 29.49	В	N
	ATOM	2082	CA	THR	116		-93.974		1.00 28.65	В	C
	MOTA	2083	CB	THR	116		-94.914		1.00 29.45	В	C
5	MOTA	2084		THR	116		-96.168		1.00 31.34	В	0
o	MOTA	2085	CG2	THR	116		-95.147		1.00 29.40	В	C
	ATOM	2086	C	THR	116		-92.658		1.00 27.59	В	C
	ATOM	2087	0	THR	116		-92.359		1.00 27.35	В	0
	ATOM	2088	N	LEU	117		-91.882		1.00 25.67	В	N
10	ATOM	2089	CA	LEU	117		-90.594		1.00 24.51	В	C
10	MOTA	2090	CB	LEU LEU	117		-89.949		1.00 22.66 1.00 23.35	В	C C
	ATOM	2091	CG	LEU	117 117		-90.544 -89.953		1.00 23.35	В	C
	ATOM ATOM	2092 2093		LEU	117		-90.261		1.00 22.38	B B	c
	ATOM	2093	CDZ	LEU	117			117.607	1.00 22.82	В	C
15	ATOM	2094	Ö	LEU	117			116.580	1.00 22.11	В	Ö
10	ATOM	2096	N	LEU	118			118.416	1.00 22.11	В	N
	ATOM	2090	CA	LEU	118			118.152	1.00 23.66	В	C
	MOTA	2098	CB	LEU	118			119.276	1.00 25.11	В	c
	ATOM	2099	CG	LEU	118			119.697	1.00 27.59	В	Č
20	ATOM	2100		LEU	118			120.242	1.00 28.18	В	č
	ATOM	2101		LEU	118			118.527	1.00 28.59	В	č
	ATOM	2102	C	LEU	118			116.827	1.00 23.33	В	Ċ
	MOTA	2103	Ō	LEU	118			116.054	1.00 22.58	В	0
	MOTA	2104	N	GLY	119			116.585	1.00 22.04	В	N
25	MOTA	2105	CA	GLY	119	16.255	-90.931	115.362	1.00 21.87	В	C
	ATOM	2106	С	GLY	119	15.491	-90.497	114.127	1.00 21.81	В	C
	MOTA	2107	0	GLY	119	16.072	-89.949	113.191	1.00 21.52	В	0
	MOTA	2108	N	ALA	120			114.122	1.00 21.37	В	N
	MOTA	2109	CA	ALA	120			113.004	1.00 21.05	В	С
30	MOTA	2110	CB	ALA	120			113.233	1.00 20.81	В	С
	MOTA	2111	С	ALA	120			112.833	1.00 21.40	В	С
	ATOM	2112	0	ALA	120			111.716	1.00 20.48	В	0
	ATOM	2113	N	HIS	121			113.945	1.00 22.14	В	N
35	ATOM	2114	CA	HIS	121			113.914	1.00 22.47	В	C
33	MOTA	2115	CB	HIS	121			115.325	1.00 22.23	B B	C
	MOTA MOTA	2116 2117	CG	HIS HIS	121 121			115.433 115.284	1.00 24.18 1.00 23.87	В	C
	ATOM	2118		HIS	121			115.657	1.00 24.73	В	N
	ATOM	2119		HIS	121			115.638	1.00 25.53	В	Č
40	ATOM	2120		HIS	121			115.413	1.00 25.90	В	N
	ATOM	2121	C	HIS	121			113.339	1.00 22.36	В	C
	ATOM	2122	Ö	HIS	121			112.448	1.00 22.60	В	ō
	ATOM	2123	N	THR	122			113.849	1.00 21.59	В	N
	ATOM	2124	CA	THR	122			113.387	1.00 21.97	В	С
45	MOTA	2125	СВ	THR	122			114.199	1.00 22.09	В	С
	MOTA	2126	OG1	THR	122	17.948	-86.364	115.561	1.00 24.17	В	0
	MOTA	2127	CG2	? THR	122	19.397	' -86.384	113.655	1.00 22.21	В	C
	MOTA	2128	С	THR	122			111.907	1.00 21.55	В	С
	MOTA	2129	0	THR	122			111.188	1.00 20.90	В	0
50	MOTA	2130		ARG	123			111.455		В	N
	MOTA	2131		ARG	123			110.063		В	С
	MOTA	2132		ARG	123			2 109.852		В	
	MOTA	2133		ARG	123			5 110.237		В	
EE	MOTA	2134		ARG	123			6 109.753 0 110 380		В	-
55	MOTA	2135		ARG	123			0 110.380 0 111 601		В	-
	MOTA	2136		ARG	123			9 111.601 2 112.352		B B	
	MOTA	2137		1 ARG	123					В	
	MOTA	2138	NH.	2 ARG	123	15.333	, -33.40	7 112.086	1.00 20.21	•	1/4

-206-

			_			16 166 07 103 100 043 1 00 20 64 7	_
	MOTA	2139		ARG	123		C
	ATOM	2140	0	ARG	123		0
	MOTA	2141	N	HIS	124		N
5	ATOM	2142		HIS	124		C
3	MOTA	2143	CB	HIS	124	12.841 -87.089 108.121 1.00 22.74 B	C
	ATOM	2144	CG	HIS	124	13.190 -88.501 107.763 1.00 23.34 B	C
	ATOM	2145	CD2		124	13.757 -89.023 106.650 1.00 22.54 B	С
	ATOM	2146	ND1		124	12.991 -89.562 108.624 1.00 22.99 B	N
40	MOTA	2147	CE1		124	13.421 -90.674 108.055 1.00 21.00 B	C
10	MOTA	2148		HIS	124	13.891 -90.375 106.858 1.00 21.93 B	N
	MOTA	2149	C	HIS	124	13.588 -84.772 108.653 1.00 23.63 B	C
	MOTA	2150	0	HIS	124	13.238 -84.069 107.700 1.00 24.39 B	0
	ATOM	2151	N	MET	125	13.589 -84.322 109.905 1.00 22.90 B	N
45	ATOM	2152	CA	MET	125	13.097 -82.976 110.197 1.00 22.76 B	С
15	ATOM	2153	CB	MET	125	11.817 -83.071 111.038 1.00 22.21 B	C
	MOTA	2154	CG	MET	125	10.710 -83.920 110.415 1.00 21.83 B	C
	MOTA	2155	SD	MET	125	9.120 -83.745 111.269 1.00 22.85 B	S
	MOTA	2156	CE	MET	125	9.499 -84.456 112.900 1.00 22.30 B	C
~~	MOTA	2157	C	MET	125	14.065 -82.015 110.880 1.00 22.78 B	C
20	MOTA	2158	0	MET	125	14.118 -80.833 110.530 1.00 22.22 B	0
	MOTA	2159	N	GLY	126	14.818 -82.527 111.852 1.00 22.55 B	N
	MOTA	2160	CA	GLY	126	15.758 -81.721 112.614 1.00 22.45 B	C
	MOTA	2161	С	GLY	126	16.466 -80.574 111.919 1.00 23.15 B	С
	MOTA	2162	0	GLY	126	16.502 -79.458 112.438 1.00 23.04 B	0
25	MOTA	2163	N	THR	127	17.047 -80.840 110.757 1.00 22.96 B	N
	MOTA	2164	CA	THR	127	17.756 -79.804 110.026 1.00 23.87 B	C
	MOTA	2165	CB	THR	127	19.261 -80.133 109.920 1.00 25.68 B	С
	ATOM	2166	OG1		127	19.417 -81.510 109.569 1.00 27.25 B	0
	MOTA	2167	CG2		127	19.969 -79.868 111.242 1.00 26.03 B	С
30	MOTA	2168	С	THR	127	17.203 -79.606 108.624 1.00 22.94 B	C
	MOTA	2169	0	THR	127	17.920 -79.166 107.728 1.00 22.72 B	0
	MOTA	2170	N	MET	128	15.927 -79.925 108.429 1.00 22.41 B	N
	MOTA	2171	CA	MET	128	15.320 -79.764 107.114 1.00 22.16 B	С
	MOTA	2172	CB	MET	128	13.897 -80.330 107.101 1.00 21.38 B	C
35	MOTA	2173	CG	MET	128	12.872 -79.579 107.943 1.00 20.15 B	C
	MOTA	2174	SD	MET	128	11.239 -80.338 107.749 1.00 20.67 B	S
	MOTA	2175	CE	MET	128	10.284 -79.362 108.917 1.00 22.56 B	С
	MOTA	2176	С	MET	128	15.305 -78.305 106.669 1.00 22.32 B	C
	ATOM	2177	0	MET	128	15.261 -78.019 105.476 1.00 22.98 B	0
40	ATOM	2178	N	PHE	129	15.363 -77.384 107.627 1.00 22.69 B	N
	MOTA	2179	CA	PHE	129	15.358 -75.957 107.311 1.00 24.34 B	С
	ATOM	2180	CB	PHE	129	15.281 -75.127 108.605 1.00 25.41 B	
	MOTA	2181	CG	PHE	129	16.565 -75.092 109.396 1.00 28.48 B	C
	MOTA	2182		PHE	129	17.588 -74.210 109.052 1.00 30.09 B	С
45	ATOM	2183		PHE	129	16.749 -75.934 110.486 1.00 29.53 B	C
	MOTA	2184		PHE	129	18.775 -74.164 109.784 1.00 31.38 B	C
	MOTA	2185	CE2		129	17.928 -75.900 111.228 1.00 31.21 B	C
	MOTA	2186	CZ	PHE	129	18.945 -75.012 110.875 1.00 32.22 B	C
	MOTA	2187	С	PHE	129	16.580 -75.540 106.485 1.00 24.09 B	C
50	MOTA	2188	0	PHE	129	16.566 -74.501 105.821 1.00 23.81 B	0
	MOTA	2189	N	GLU	130	17.636 -76.346 106.522 1.00 24.21 B	N
	MOTA	2190	CA	GLU	130	18.843 -76.031 105.762 1.00 25.33 B	C
	MOTA	2191	СВ	GLU	130	20.011 -76.906 106.222 1.00 27.28 B	C
	MOTA	2192		GLU	130	20.376 -76.718 107.685 1.00 31.35 B	C
55	ATOM	2193	CD	GLU	130	21.694 -77.377 108.045 1.00 34.28 B	C
	MOTA	2194		l GLU	130	22.057 -78.381 107.389 1.00 35.08 B	0
	MOTA	2195		GLU	130	22.360 -76.898 108.992 1.00 36.90 B	0
	MOTA	2196	С	GLU	130	18.647 -76.197 104.258 1.00 23.24 B	C

-207-

	ATOM	2197	0	GLU	130	9.439 -75.686 103.470	1.00 23.56	В	0
	ATOM	2198	N	GLN	131	7.601 -76.918 103.865	1.00 21.55	В	N
	MOTA	2199	CA	GLN	131	7.302 -77.125 102.453	1.00 20.76	В	С
	MOTA	2200	CB	GLN	131	6.539 -78.442 102.240	1.00 21.85	В	С
5	ATOM	2201	CG	GLN	131	7.320 -79.703 102.536	1.00 23.34	В	С
	ATOM	2202	CD	GLN	131	8.691 -79.696 101.882	1.00 26.07	В	C
	MOTA	2203	OE1	GLN	131	8.815 -79.538 100.664	1.00 26.66	В	0
	ATOM	2204	NE2	GLN	131	9.728 -79.862 102.692	1.00 26.55	В	N
	MOTA	2205	С	GLN	131	6.462 -75.987 101.869	1.00 20.02	В	С
10	ATOM	2206	0	GLN	131	6.346 -75.875 100.659	1.00 20.04	В	0
	ATOM	2207	N	PHE	132	15.880 -75.149 102.724	1.00 19.42	В	N
	ATOM	2208	CA	PHE	132	15.023 -74.048 102.269	1.00 19.05	В	C
	ATOM	2209	CB	PHE	132	4.612 -73.157 103.454	1.00 17.06	В	C
	ATOM	2210	CG	PHE	132	13.572 -73.779 104.384	1.00 16.44	В	C
15	ATOM	2211		PHE	132	13.055 -75.055 104.152	1.00 15.33	В	C
	ATOM	2212		PHE	132	13.117 -73.073 105.493	1.00 15.55	В	С
	ATOM	2213		PHE	132	12.099 -75.620 105.018	1.00 15.93	В	C
	ATOM	2214	CE2		132	12.157 -73.626 106.368	1.00 15.23	В	C
	ATOM	2215	CZ	PHE	132	11.651 -74.895 106.132	1.00 15.15	В	C
20	ATOM	2216	c	PHE	132	15.650 -73.182 101.170	1.00 19.75	В	Ċ
	ATOM	2217	ō	PHE	132	14.957 -72.736 100.254	1.00 19.12	В	0
	ATOM	2218	N	VAL	133	16.955 -72.946 101.266	1.00 20.25	В	N
	ATOM	2219	CA	VAL	133	17.675 -72.139 100.287	1.00 21.53	В	C
	ATOM	2220	СВ	VAL	133	19.135 -71.915 100.737	1.00 22.78	В	Ċ
25	ATOM	2221		VAL	133	19.901 -73.236 100.711	1.00 21.70	В	Ċ
	ATOM	2222		VAL	133	19.799 -70.870 99.850	1.00 23.73	В	Ċ
	ATOM	2223	C	VAL	133	17.673 -72.750 98.877	1.00 22.37	В	C
	ATOM	2224	ō	VAL	133	17.955 -72.058 97.895	1.00 21.91	В	ō
	ATOM	2225	N	GLN	134	17.344 -74.036 98.780	1.00 22.29	В	N
30	ATOM	2226	CA	GLN	134	17.294 -74.725 97.496	1.00 23.37	В	C
	ATOM	2227	СВ	GLN	134	17.558 -76.229 97.680	1.00 22.92	В	C
	ATOM	2228	CG	GLN	134	18.860 -76.621 98.407	1.00 23.40	В	Č
	ATOM	2229	CD	GLN	134	20.154 -76.250 97.659	1.00 23.05	В	C
	ATOM	2230	OE1		134	21.237 -76.701 98.020	1.00 25.27	В	Ō
35	ATOM	2231	NE2		134	20.042 -75.430 96.639	1.00 22.55	В	N
	ATOM	2232	C	GLN	134	15.954 -74.548 96.768		В	C
	ATOM	2233	ō	GLN	134	15.771 -75.081 95.678		В	0
	ATOM	2234	N	PHE	135	15.022 -73.804 97.361		В	N
	ATOM	2235	CA	PHE	135	13.710 -73.595 96.750		В	С
40	ATOM	2236	СВ	PHE	135	12.626 -74.065 97.722		В	C
. •	ATOM	2237	CG	PHE	135	12.706 -75.534 98.039		В	C
	ATOM	2238	CD1		135	12.206 -76.478 97.146		В	C
	MOTA	2239		PHE	135	13.335 -75.977 99.198		В	C
	ATOM	2240		PHE	135	12.331 -77.848 97.397		В	C
45	ATOM	2241		PHE	135	13.470 -77.349 99.466		В	C
	ATOM	2242	CZ	PHE	135	12.966 -78.286 98.560		В	С
	ATOM	2243	C	PHE	135	13.500 -72.130 96.358		В	С
	ATOM	2244	o	PHE	135	12.508 -71.501 96.739		В	0
	ATOM	2245	N	ARG	136	14.444 -71.622 95.566		В	N
50	ATOM	2246	CA	ARG	136	14.486 -70.241 95.098		В	С
	MOTA	2247	СВ	ARG	136	14.046 -70.118 93.626		В	C
	ATOM	2248	CG	ARG	136	12.754 -70.801 93.245		В	
	MOTA	2249	CD	ARG	136	13.002 -72.190 92.685		В	
	ATOM	2250	NE	ARG	136	11.998 -73.127 93.184		В	
55	ATOM	2251	CZ	ARG	136	12.120 -74.448 93.158		В	
	ATOM	2252		1 ARG	136	13.214 -75.011 92.649		В	
	ATOM	2253		2 ARG	136	11.152 -75.207 93.654		В	
	ATOM	2254		ARG	136	13.765 -69.204 95.951			
	111014	2234	_		150			_	~

-208-

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	MOTA	2255		ARG	136	12.679		95.618	1.00 27.33		0
	MOTA	2256	N	PRO	137	14.379		97.085	1.00 28.01		N
	MOTA	2257	CD	PRO	137	15.580		97.667	1.00 27.43		C
_	ATOM	2258	CA	PRO	137		-67.860	97.999	1.00 27.65		C
5	MOTA	2259	СВ	PRO	137	14.586		99.286	1.00 27.04		C
	MOTA	2260	CG	PRO	137		-68.518	98.778	1.00 27.95		C
	MOTA	2261	C	PRO	137		-66.467	97.451	1.00 27.46		C
	MOTA	2262	0	PRO	137		-66.190	96.981	1.00 27.51		0
40	MOTA	2263	N	PRO	138		-65.578	97.479	1.00 26.95		N
10	MOTA	2264	CD	PRO	138		-65.734	97.852	1.00 26.96		C
	ATOM	2265	CA	PRO	138		-64.234	96.968	1.00 26.24		C
	MOTA	2266	CB	PRO	138	12.051	-63.496	97.228	1.00 26.54	В	C
	MOTA	2267	CG	PRO	138		-64.341	98.273	1.00 27.40	В	С
	MOTA	2268	С	PRO	138	14.573	-63.608	97.679	1.00 25.08	В	С
15	MOTA	2269	0	PRO	138	14.928	-63.992	98.799	1.00 23.40	В	0
	MOTA	2270	N	ALA	139	15.194	-62.642	97.014	1.00 24.45	В	N
	ATOM	2271	CA	ALA	139	16.377	-61.959	97.529	1.00 24.74	В	C
	MOTA	2272	CB	ALA	139	16.852	-60.925	96.503	1.00 25.14		С
	ATOM	2273	С	ALA	139	16.283	-61.300	98.905	1.00 24.49		C
20	ATOM	2274	0	ALA	139	17.268	-61.293	99.651	1.00 24.23		0
	ATOM	2275	N	HIS	140		-60.749	99.252	1.00 24.55		N
	ATOM	2276	CA	HIS	140		-60.066		1.00 24.29		C
	MOTA	2277	CB	HIS	140		-59.245		1.00 23.87		Ċ
	ATOM	2278	CG	HIS	140		-60.056		1.00 23.38		Č
25	MOTA	2279		HIS	140		-60.232		1.00 23.33		C
	ATOM	2280		HIS	140		-60.783	99.833	1.00 23.88		N
	ATOM	2281		HIS	140		-61.371	100.328	1.00 24.03		C
	ATOM	2282		HIS	140		-61.054		1.00 24.40		N
	MOTA	2283	С	HIS	140		-60.951		1.00 24.3		C
30	ATOM	2284	0	HIS	140		-60.439		1.00 24.0		0
	ATOM	2285	N	LEU	141	15.010	-62.265	101.605	1.00 24.49		N
	ATOM	2286	CA	LEU	141	15.117	-63.216	102.714	1.00 25.6		C
	ATOM	2287	CB	LEU	141	14.436	-64.544	102.352	1.00 24.5	2 B	C
	ATOM	2288	CG	LEU	141	12.951	-64.562	101.981	1.00 25.1	4 B	С
35	ATOM	2289	CD1	LEU	141	12.529	-65.992	101.647	1.00 23.5	2 B	С
	ATOM	2290	CD2	LEU	141	12.118	-64.006	103.143	1.00 23.7	3 B	С
	ATOM	2291	С	LEU	141	16.577	-63.512	103.056	1.00 26.6	2 в	С
	ATOM	2292	0	LEU	141	16.886	-64.005	104.138	1.00 26.3		0
	MOTA	2293	N	PHE	142			102.130	1.00 28.4		N
40	ATOM	2294	CA	PHE	142	18.888	-63.495	102.331	1.00 31.8	2 B	C
	ATOM	2295	СВ	PHE	142		-63.519		1.00 29.2		C
	ATOM	2296	CG	PHE	142			100.212			
	ATOM	2297		PHE	142			100.393	1.00 25.1		
	ATOM	2298		PHE	142			99.331	1.00 26.5		
45	MOTA	2299		PHE	142		-67.056		1.00 25.7		C
	ATOM	2300		PHE	142	18.093	-66.074	98.639	1.00 26.2		C
	ATOM	2301	CZ	PHE	142		-67.159		1.00 25.2		C
	MOTA	2302	C	PHE	142			103.275	1.00 35.2		
	ATOM	2303	0	PHE	142			103.281	1.00 35.5		
50	MOTA	2304	N	ILE	143			104.071	1.00 39.0		
	ATOM	2305	CA	ILE	143			105.028	1.00 42.7		-
	MOTA	2306	CB	ILE	143			104.472	1.00 42.5		
	ATOM	2307		ILE	143			105.529	1.00 42.5		
	ATOM	2308		ILE	143			104.032	1.00 42.8		
55	ATOM	2309		ILE	143			103.438	1.00 43.3		
	ATOM	2310		ILE	143			105.388	1.00 45.2		
	ATOM	2311	Ö	ILE	143			106.333	1.00 46.1		
	ATOM	2312		HIS	144			104.636	1.00 48.1		
	011								40.1	۔ ۔	*4

WO 2005/019239 PCT/US2004/023092

-209-

	3.0004	2212	01		144	21 120	-58.766	104 005	1.00 50.43	_	^
	ATOM	2313	CA CB	HIS HIS	144		-58.077		1.00 50.43	В	C
	ATOM	2314								В	C
	MOTA	2315	CG	HIS	144		-58.553	106.941	1.00 53.18	В	
5	MOTA	2316	CD2		144			107.873	1.00 53.68	В	C
3	ATOM	2317	ND1		144			107.520	1.00 53.87	В	N
	MOTA	2318	CE1		144	23.843	-58.939	108.747	1.00 53.89	В	C
	ATOM	2319	NE2		144	22.613		108.985	1.00 53.40	В	N
	MOTA	2320	С	HIS	144	20.688	-58.010	103.655	1.00 50.90	В	С
	ATOM	2321	0	HIS	144	21.479	-57.322	103.006	1.00 51.65	В	0
10	MOTA	2322	N	HIS	145	19.403	-58.149	103.339	1.00 51.36	В	N
	ATOM	2323	CA	HIS	145	18.778	-57.503	102.183	1.00 51.48	В	C
	ATOM	2324	CB	HIS	145	18.251	-58.577	101.223	1.00 52.46	В	C
	ATOM	2325	CG	HIS	145	18.066	-58.105	99.812	1.00 53.73	В	C
	ATOM	2326		HIS	145		-57.714	99.140	1.00 54.04	В	C
15	ATOM	2327		HIS	145		-58.015	98.915	1.00 54.94	В	N
	ATOM	2328		HIS	145		-57.592	97.750	1.00 54.82	В	C
	ATOM	2329		HIS	145		-57.401	97.859	1.00 54.54	В	N
	ATOM	2330	C	HIS	145		-56.629		1.00 50.58	В	C
	ATOM	2331	Ö	HIS	145		-56.929		1.00 50.62	В	Ö
20				GLN	146		-55.552	101.950	1.00 30.02	В	N
20	ATOM	2332	N								
	ATOM	2333	CA	GLN	146		-54.650		1.00 48.58	В	C
	ATOM	2334	CB	GLN	146		-53.426		1.00 50.29	В	C
	MOTA	2335	CG	GLN	146		-52.329		1.00 52.37	В	C
05	ATOM	2336	CD	GLN	146			100.661	1.00 53.97	В	C
25	ATOM	2337		GLN	146		-52.395		1.00 55.36	В	0
	ATOM	2338	NE2		146			101.172	1.00 53.39	В	N
	MOTA	2339	C	GLN	146			102.152	1.00 46.43	В	С
	ATOM	2340	0	GLN	146	14.772	-56.250	101.259	1.00 47.01	В	0
	MOTA	2341	N	PRO	147	13.906	-55.140	103.024	1.00 43.87	В	N
30	MOTA	2342	CD	PRO	147	13.896	-54.126	104.094	1.00 42.94	В	C
	ATOM	2343	CA	PRO	147	12.604	-55.823	102.952	1.00 40.85	В	С
	ATOM	2344	CB	PRO	147	11.805	-55.171	104.081	1.00 41.31	В	C
	ATOM	2345	CG	PRO	147			104.211	1.00 42.30	В	С
	ATOM	2346	C	PRO	147		-55.697		1.00 37.44	В	C
35	ATOM	2347	ō	PRO	147			100.733	1.00 36.62	В	0
	ATOM	2348	N	LEU	148			101.408	1.00 34.45	В	N
	ATOM	2349	CA	LEU	148			100.143	1.00 31.79	В	Ĉ
	ATOM	2350	СВ	LEU	148			100.162	1.00 30.82	В	Č
	ATOM	2351	CG	LEU	148		-58.528		1.00 30.02	В	Č
40	ATOM	2352		LEU	148		-58.918		1.00 30.58	В	C
70		2352		LEU	148		-58.102		1.00 30.38	В	C
	ATOM								1.00 30.13	В	C
	ATOM	2354	C	LEU	148		-55.018				
	MOTA	2355	0	LEU	148			100.653	1.00 28.77	В	0
AE	MOTA	2356	N	PRO	149		-54.448		1.00 27.64	В	N
45	MOTA	2357	CD	PRO	149		-54.900		1.00 27.10	В	C
	MOTA	2358	CA	PRO	149		-53.114		1.00 26.65	В	С
	MOTA	2359	СВ	PRO	149		-52.829		1.00 26.71	В	C
	MOTA	2360	CG	PRO	149		-53.593		1.00 26.43	В	С
	MOTA	2361	С	PRO	149	7.833	-53.103		1.00 25.49	В	C
50	MOTA	2362	0	PRO	149		-54.132		1.00 25.29	В	0
	MOTA	2363	N	THR	150	7.248	-51.932	98.516	1.00 24.33	В	N
	ATOM	2364	CA	THR	150	5.799	-51.782	2 98.494	1.00 23.46	В	C
	ATOM	2365	CB	THR	150		-50.28		1.00 23.36	В	
	ATOM	2366		LTHR	150		-49.84				
55	ATOM	2367		2 THR	150		-50.07				
	ATOM	2368		THR	150		-52.35				
	ATOM	2369		THR	150		-53.05				
	ATOM	2370		LEU	151		-52.07				
	AIOM	23/0	14	LEU	171	5.071	-32.07	, ,,,,,,	1.00 23.33	٥	TA

-210-

	MOTA	2371	CA	LEU	151	5.086 -5		94.818	1.00 24.18	В	С
	MOTA	2372		LEU	151	5.174 -		93.764	1.00 23.98	В	C
	MOTA	2373		LEU	151	3.943 -		93.516	1.00 26.19	В	C
_	MOTA	2374	CD1		151	3.125 -		94.783	1.00 25.29	В	C
5	MOTA	2375		LEU	151	4.406 -4		92.956	1.00 25.33	В	C
	MOTA	2376	C	LEU	151	5.692 -		94.256	1.00 24.80	В	C
	MOTA	2377	0	LEU	151	5.289 -		93.188	1.00 24.09	В	0
	MOTA	2378	N	ALA	152	6.651 -		94.965	1.00 25.14	В	N
40	ATOM	2379	CA	ALA	152	7.269 -		94.485	1.00 25.42	В	С
10	MOTA	2380	CB	ALA	152	8.449 -		95.357	1.00 25.27	В	С
	MOTA	2381	C	ALA	152	6.255 -		94.483	1.00 25.45	В	C
	MOTA	2382	0	ALA	152	5.516 -		95.447	1.00 26.33	В	0
	ATOM	2383	N	PRO	153	6.182 -		93.385	1.00 25.59	В	N
15	ATOM	2384	CD	PRO	153	6.844 -		92.078	1.00 26.03	В	C
15	ATOM	2385	CA	PRO	153	5.214 -		93.373	1.00 25.15	В	C
	ATOM	2386	CB	PRO	153	5.337 -		91.953	1.00 25.93	В	C
	ATOM	2387	CG	PRO	153	6.712 -		91.514	1.00 27.37	В	C
	ATOM	2388	C	PRO	153	5.538 -		94.457	1.00 24.29	В	C
20	MOTA	2389	0	PRO	153	6.705 -		94.776	1.00 23.77	В	0
20	ATOM	2390	N	VAL	154	4.502 -		95.031	1.00 23.14	В	N
	MOTA	2391	CA CB	VAL	154	4.689 -		96.090	1.00 23.20 1.00 23.14	В	C
	MOTA MOTA	2392 2393	-	VAL VAL	154 154	3.612 - 3.638 -		97.205		В	C
	ATOM	2394		VAL	154	2.233 -		97.761 96.656	1.00 24.25 1.00 22.99	В	C
25	MOTA	2395	C	VAL	154	4.669 -		95.589	1.00 22.99	B B	C
20	ATOM	2396	Ö	VAL	154	4.882 -		96.364	1.00 22.02	В	0
	ATOM	2397	N	LEU	155	4.413 -		94.298	1.00 21.04	В	N
	ATOM	2398	CA	LEU	155	4.374 -		93.711	1.00 21.77	В	C
	ATOM	2399	CB	LEU	155	4.170 -		92.191	1.00 21.77	В	C
30	ATOM	2400	CG	LEU	155	4.166 -		91.410	1.00 22.05	В	C
•	ATOM	2401		LEU	155	3.033 -		91.892	1.00 20.48	В	Č
	ATOM	2402		LEU	155	4.017 -		89.905	1.00 22.31	В	C
	ATOM	2403	C	LEU	155	5.622		94.030	1.00 20.95	В	Č
	ATOM	2404	ŏ	LEU	155	5.496 -		94.373	1.00 21.26	В	o
35	ATOM	2405	N	PRO	156	6.838 -		93.908	1.00 20.25	В	N
	ATOM	2406	CD	PRO	156	7.210 -		93.313	1.00 20.55	В	C
	ATOM	2407	CA	PRO	156	8.040 -		94.218	1.00 20.02	В	C
	ATOM	2408	СВ	PRO	156	9.178 -		93.942	1.00 19.60	В	C
	ATOM	2409	CG	PRO	156	8.627 -	63.462	92.821	1.00 19.34	В	С
40	ATOM	2410	C	PRO	156	8.043 -	-65.793	95.675	1.00 20.44	В	C
	MOTA	2411	0	PRO	156	8.401 -		95.948	1.00 18.86	В	0
	MOTA	2412	N	LEU	157	7.646 -		96.603	1.00 18.95	В	N
	ATOM	2413	CA	LEU	157	7.584 -		98.012	1.00 18.72	В	C
	MOTA	2414	CB	LEU	157	7.243 -		98.886	1.00 18.06	В	С
45	ATOM	2415	CG	LEU	157			100.390	1.00 18.20	В	C
	MOTA	2416		LEU	157			100.910	1.00 18.30	В	C
	MOTA	2417		LEU	157			101.133	1.00 18.86	В	C
	MOTA	2418	C	LEU	157		-66.376	98.210	1.00 18.16	В	C
50	MOTA	2419	0	LEU	157		-67.369	98.892	1.00 17.47	В	0
50	ATOM	2420	N	VAL	158		-66.174	97.612	1.00 17.84	В	N
	MOTA	2421	CA	VAL	158		-67.132	97.713	1.00 18.75	В	С
	MOTA	2422	CB	VAL	158		-66.637	96.928	1.00 19.19	В	C
	ATOM	2423		VAL	158		-67.746	96.840	1.00 18.53	В	C
EE	ATOM	2424		VAL	158		-65.397	97.610	1.00 19.01	В	C
55	MOTA	2425	C	VAL	158		-68.504	97.167	1.00 19.26	В	C
	MOTA	2426	0	VAL	158		-69.539	97.773	1.00 17.72	В	0
	ATOM	2427	N	THR	159		-68.504	96.009	1.00 19.18	В	N
	MOTA	2428	CA	THR	159	5./49	-69.742	95.382	1.00 20.12	В	C

-211-

	MOTA	2429	СВ	THR	159	6.359	-69.464	94.005	1.00 20.73	В	С
	MOTA	2430	OG1	THR	159		-68.696	93.233	1.00 21.98	В	0
	MOTA	2431	CG2	THR	159	6.670	-70.780	93.277	1.00 20.98	В	C
_	MOTA	2432	С	THR	159		-70.418	96.270	1.00 19.12	В	C
5	ATOM	2433	0	THR	159	6.757	-71.631	96.447	1.00 19.81	В	0
	MOTA	2434	N	HIS	160	7.695	-69.624	96.827	1.00 18.60	В	N
	MOTA	2435	ÇA	HIS	160	8.725	-70.143	97.722	1.00 19.62	В	C
	MOTA	2436	CB	HIS	160	9.628	-69.004	98.201	1.00 19.12	В	C
	MOTA	2437	CG	HIS	160	10.583	-69.405	99.283	1.00 20.97	В	C
10	MOTA	2438	CD2	HIS	160	10.739	-68.946	100.548	1.00 19.99	В	C
	ATOM	2439	ND1	HIS	160		-70.374	99.106	1.00 21.00	В	N
	MOTA	2440	CE1	HIS	160	12.258	-70.492	100.214	1.00 20.06	В	C
	MOTA	2441	NE2		160	11.787	-69.637	101.103	1.00 18.80	В	N
	ATOM	2442	С	HIS	160	8.069	-70.835	98.922	1.00 18.85	В	C
15	MOTA	2443	0	HIS	160	8.465	-71.934	99.309	1.00 19.48	В	0
	MOTA	2444	N	PHE	161	7.065	-70.192	99.510	1.00 18.30	В	N
	MOTA	2445	CA	PHE	161	6.362	-70.783	100.644	1.00 17.81	В	C
	ATOM	2446	ÇВ	PHE	161	5.333	-69.799	101.218	1.00 17.09	В	C
	MOTA	2447	CG	PHE	161	5.924	-68.773	102.167	1.00 18.77	В	C
20	MOTA	2448	CD1	PHE	161	7.253	-68.861	102.576	1.00 18.08	В	C
	MOTA	2449	CD2	PHE	161	5.137	-67.743	102.675	1.00 18.45	В	C
	MOTA	2450	CE1	PHE	161	7.788	-67.943	103.478	1.00 19.86	В	C
	MOTA	2451	CE2	PHE	161	5.658	-66.818	103.577	1.00 19.78	В	C
	ATOM	2452	CZ	PHE	161	6.992	-66.918	103.981	1.00 20.06	В	C
25	ATOM	2453	C	PHE	161	5.675	-72.081	100.227	1.00 17.47	В	С
	MOTA	2454	0	PHE	161	5.721	-73.075	100.953	1.00 16.02	В	0
	MOTA	2455	N	ALA	162	5.039	-72.082	99.058	1.00 16.64	В	N
	ATOM	2456	CA	ALA	162	4.361	-73.286	98.588	1.00 17.85	В	C
	ATOM	2457	CB	ALA	162	3.712	-73.034	97.224	1.00 17.30	В	C
30	MOTA	2458	C	ALA	162	5.352	-74.447	98.487	1.00 18.28	В	С
	MOTA	2459	0	ALA	162	5.055	-75.563	98.899	1.00 17.59	В	0
	MOTA	2460	N	ASP	163	6.530	-74.166	97.935	1.00 18.81	В	N
	ATOM	2461	CA	ASP	163	7.569	-75.170	97.763	1.00 20.29	В	C
	MOTA	2462	CB	ASP	163		-74.624		1.00 21.76	В	C
35	ATOM	2463	CG	ASP	163		-74.448		1.00 22.93	В	C
	MOTA	2464		ASP	163		-73.763		1.00 25.09	В	0
	MOTA	2465	OD2	ASP	163		-75.005		1.00 23.14	В	0
	MOTA	2466	C	ASP	163		-75.671		1.00 20.12	В	C
4.0	MOTA	2467	0	ASP	163		-76.873		1.00 18.59	В	0
40	MOTA	2468	N	ILE	164		-74.780		1.00 19.96	В	N
	MOTA	2469	CA	ILE	164			101.240	1.00 20.35	В	С
	ATOM	2470	CB	ILE	164			102.071	1.00 20.04	В	_
	MOTA	2471		ILE	164			101.224	1.00 19.12	В	С
45	MOTA	2472		ILE	164			102.555	1.00 20.01	В	C
45	MOTA	2473		ILE	164			103.497	1.00 18.11	В	C
	MOTA	2474	C	ILE	164			102.076	1.00 20.60	В	C
	MOTA	2475	0	ILE	164			102.819	1.00 20.54	В	0
	ATOM	2476	N	ASN	165			101.939	1.00 19.91	В	N
E0	MOTA	2477	CA	ASN	165			102.673	1.00 19.83	В	С
50	MOTA	2478	CB	ASN	165			102.464	1.00 18.46	В	С
	MOTA	2479	CG	ASN	165			103.244	1.00 19.03	В	C
	ATOM	2480		ASN	165			104.145		В	0
	ATOM	2481		2 ASN	165			102.900		В	N
	ATOM	2482	C	ASN	165			102.174		В	C
55	ATOM	2483	0	ASN	165			102.960		В	0
	MOTA	2484	N	THR	166			100.859		В	N
	MOTA	2485		THR	166			100.279		В	-
	MOTA	2486	CB	THR	166	5.359	78.981	98.741	1.00 21.41	В	С

-212-

	MOTA	2487	0G1		166		-78.224		1.00 22.00	В	0
	MOTA	2488		THR	166		-80.368	98.104	1.00 20.43	В	C
	MOTA	2489	C	THR	166		-79.947		1.00 20.47	В	C
_	MOTA	2490	0	THR	166		-81.079		1.00 19.94	В	0
5	MOTA	2491	N	PHE	167		-79.403		1.00 19.96	В	N
	MOTA	2492	CA	PHE	167		-80.099		1.00 20.53	В	C
	MOTA	2493	CB	PHE	167		-79.166		1.00 20.58	В	C
	MOTA	2494	CG	PHE	167		-79.620		1.00 21.61	В	С
40	MOTA	2495	CD1		167		-80.739		1.00 21.76	В	C
10	MOTA	2496		PHE	167		-78.909		1.00 20.70	В	C
	ATOM	2497	CE1	PHE	167		-81.145		1.00 22.38	В	C
	MOTA	2498	CE2	PHE	167		-79.303		1.00 22.67	В	C
	ATOM	2499	CZ	PHE	167			103.137	1.00 22.67	В	C
	MOTA	2500	С	PHE	167			102.592	1.00 20.25	В	C
15	MOTA	2501	0	PHE	167	9.011	-81.730	102.904	1.00 20.74	В	0
	MOTA	2502	N	MET	168	8.403	-79.640	103.479	1.00 18.80	В	N
	MOTA	2503	CA	MET	168	8.235	-79.971	104.897	1.00 18.84	В	C
	MOTA	2504	CB	MET	168	7.858	-78.722	105.712	1.00 17.54	В	C
	ATOM	2505	CG	MET	168	9.004	-77.727	105.904	1.00 16.54	В	C
20	MOTA	2506	SD	MET	168	8.609	-76.401	107.082	1.00 16.62	В	S
	ATOM	2507	CE	MET	168	7.812	-75.178	106.019	1.00 15.56	В	C
	ATOM	2508	С	MET	168	7.215	-81.078	105.163	1.00 18.68	В	C
	ATOM	2509	0	MET	168	7.461	-81.969	105.970	1.00 17.64	В	0
	MOTA	2510	N	VAL	169	6.065	-81.024	104.503	1.00 19.45	В	N
25	ATOM	2511	CA	VAL	169			104.702	1.00 20.76	В	C
	MOTA	2512	CB	VAL	169			103.889	1.00 21.33	В	C
	MOTA	2513		VAL	169			103.936	1.00 20.85	В	Ċ
	ATOM	2514		VAL	169			104.458	1.00 21.08	В	Ċ
	ATOM	2515	C	VAL	169			104.275	1.00 21.26	В	Č
30	ATOM	2516	Ō	VAL	169			104.965	1.00 20.54	В	ō
	MOTA	2517	N	LEU	170			103.139	1.00 21.18	В	N
	ATOM	2518	CA	LEU	170			102.659	1.00 21.80	В	C
	ATOM	2519	СВ	LEU	170			101.338	1.00 22.86	В	č
	ATOM	2520	CG	LEU	170			100.139	1.00 24.31	В	č
35	ATOM	2521		LEU	170		-83.710		1.00 24.24	В	č
	ATOM	2522		LEU	170		-85.300		1.00 24.97	В	č
	ATOM	2523	c	LEU	170			103.702	1.00 21.40	В	Č
	ATOM	2524	ō	LEU	170			103.891	1.00 20.50	В	ŏ
	ATOM	2525	N	GLN	171			104.371	1.00 20.25	В	И
40	ATOM	2526	CA	GLN	171			105.402	1.00 20.37	В	C
	ATOM	2527	CB	GLN	171			105.808	1.00 18.76	В	Ċ
	ATOM	2528	CG	GLN	171			104.719	1.00 17.74	В	
	ATOM	2529	CD	GLN	171			104.254	1.00 18.92	В	c
	ATOM	2530		GLN	171			105.034	1.00 20.91	В	o
45	ATOM	2531		GLN	171			102.987	1.00 17.61	В	N
	ATOM	2532	C	GLN	171			106.626	1.00 20.12	В	C
	ATOM	2533	Ö	GLN	171			107.249	1.00 20.12	В	o
	ATOM	2534	N	VAL	172			106.971	1.00 19.83	В	N
	ATOM	2535	CA	VAL	172			108.112	1.00 20.71	В	C
50	ATOM	2536	CB	VAL	172			108.112	1.00 21.73	В	
30											C
	ATOM	2537		VAL	172			109.384	1.00 22.67	В	C
	ATOM	2538		VAL	172			108.874	1.00 22.87	В	C
	ATOM	2539	C	VAL	172			107.853	1.00 21.64	В	C
55	ATOM	2540	0	VAL	172			108.755	1.00 20.64	В	0
33	ATOM	2541	N	ILE	173			106.612	1.00 21.03	В	N
	ATOM	2542	CA	ILE	173			106.219	1.00 21.75	В	C
	MOTA	2543	CB	ILE	173			104.725	1.00 21.85	В	
	MOTA	2544	CG2	ILE	173	4.791	89.563	3 104.271	1.00 22.44	В	С

-213-

	MOTA	2545	CG1	ILE	173	3.908	-87.222	104.561	1.00 21.48	В	C
	ATOM	2546	CD1	ILE	173	3.360	-87.129	103.143	1.00 20.80	В	C
	MOTA	2547	C	ILE	173	6.725	-89.126	106.449	1.00 21.99	В	C
	MOTA	2548	0	ILE	173	6.512	-90.212	106.986	1.00 20.98	В	0
5	ATOM	2549	N	LYS	174	7.942	-88.742	106.057	1.00 22.27	В	N
	MOTA	2550	CA	LYS	174	9.117	-89.596	106.252	1.00 22.72	В	C
	ATOM	2551	CB	LYS	174			105.671	1.00 23.87	В	C
	ATOM	2552	CG	LYS	174			104.171	1.00 27.23	В	C
	MOTA	2553	CD	LYS	174			103.704	1.00 29.56	В	c
10	ATOM	2554	CE	LYS	174			102.342	1.00 32.40	В	Ċ
-	ATOM	2555	NZ	LYS	174			102.435	1.00 34.29	В	N
	ATOM	2556	C	LYS	174			107.743	1.00 21.87	В	c
	ATOM	2557	ō	LYS	174		-91.007		1.00 20.46	В	ŏ
	ATOM	2558	N	PHE	175			108.563	1.00 21.53	В	N
15	ATOM	2559	CA	PHE	175			110.008	1.00 21.67	В	C
.•	ATOM	2560	СВ	PHE	175			110.643	1.00 21.39	В	c
	ATOM	2561	CG	PHE	175			112.134	1.00 22.55	В	c
	ATOM	2562		PHE	175			112.995	1.00 21.38	В	c
	ATOM	2563		PHE	175			112.679	1.00 21.38	В	C
20	ATOM	2564		PHE	175			114.374	1.00 21.89	В	C
	ATOM	2565	CE2	PHE	175			114.061	1.00 23.00	В	Ċ
	ATOM	2566	CZ	PHE	175			114.910	1.00 22.35	В	C
	ATOM	2567	C	PHE	175			110.581	1.00 21.68	В	Ç
	ATOM	2568	ŏ	PHE	175			111.362	1.00 21.47	В	ŏ
25	ATOM	2569	N	THR	176			110.188	1.00 22.73	В	N
	ATOM	2570	CA	THR	176			110.686	1.00 24.75	В	C
	ATOM	2571	СВ	THR	176			110.230	1.00 25.26	В	č
	ATOM	2572	OG1		176			108.820	1.00 24.98	В	ŏ
	ATOM	2573	CG2	THR	176			110.565	1.00 24.45	В	Č
30	ATOM	2574	C	THR	176			110.257	1.00 25.69	В	č
	ATOM	2575	ō	THR	176			111.065	1.00 24.44	В	ō
	ATOM	2576	N	LYS	177			109.005	1.00 26.56	В	N
	ATOM	2577	CA	LYS	177			108.489	1.00 28.90	В	C
	MOTA	2578	СВ	LYS	177			106.958	1.00 29.06	В	C
35	ATOM	2579	CG	LYS	177			106.327	1.00 31.35	В	C
	ATOM	2580	CD	LYS	177			104.815	1.00 33.93	В	C
	MOTA	2581	CE	LYS	177			104.191	1.00 35.45	В	C
	MOTA	2582	NZ	LYS	177	3.233	-93.686	104.749	1.00 36.90	В	N
	ATOM	2583	С	LYS	177	8.265	-94.500	109.047	1.00 29.97	В	С
40	ATOM	2584	0	LYS	177	8.581	-95.632	108.681	1.00 30.08	В	0
	ATOM	2585	N	ASP	178	8.979	-93.799	109.924	1.00 30.95	В	N
	ATOM	2586	CA	ASP	178	10.171	-94.338	110.580	1.00 31.86	В	С
	ATOM	2587	CB	ASP	178	11.249	-93.255	110.695	1.00 33.44	В	С
	MOTA	2588	CG	ASP	178	12.365	-93.427	109.689	1.00 35.31	В	С
45	MOTA	2589	OD1	ASP	178	12.105	-93.955	108.587	1.00 36.42	В	0
	ATOM	2590	OD2	ASP	178	13.506	-93.018	109.994	1.00 37.36	В	0
	MOTA	2591	С	ASP	178	9.770	-94.814	111.986	1.00 31.51	В	C
	MOTA	2592	0	ASP	178	10.600	-95.282	112.760	1.00 31.62	В	0
	ATOM	2593	N	LEU	179	8.485	-94.689	112.299	1.00 31.35	В	N
50	MOTA	2594	CA	LEU	179	7.945	-95.083	113.593	1.00 31.19	В	C
	MOTA	2595	CB	LEU	179			114.136	1.00 31.02	В	C
	MOTA	2596	CG	LEU	179			114.840	1.00 31.99	В	C
	ATOM	2597		LEU	179			7 114.255	1.00 31.68	В	С
	ATOM	2598	CD2	LEU	179	6.650	-91.592	2 114.747	1.00 31.31	В	C
55	MOTA	2599	C	LEU	179	7.127	-96.358	3 113.425	1.00 31.91	В	С
	MOTA	2600		LEU	179			3 112.923	1.00 30.72	В	0
	MOTA	2601	N	PRO	180			3 113.844		В	
	MOTA	2602	CD	PRO	180	8.944	-97.73	l 114.565	1.00 32.93	В	С

-214-

	MOTA	2603	CA	PRO	180	6.932 -98.758 113.700 1.00 33.57 B	C
	MOTA	2604	СВ	PRO	180	7.842 -99.789 114.374 1.00 33.58 B	C
	MOTA	2605	CG	PRO	180	8.636 -98.981 115.341 1.00 33.83 B	C
_	ATOM	2606	C	PRO	180	5.535 -98.679 114.319 1.00 34.14 B	C
5	MOTA	2607	0	PRO	180	4.569 -99.203 113.763 1.00 33.78 B	0
	ATOM	2608	N	VAL	181	5.427 -98.002 115.457 1.00 34.64 B	N
	MOTA	2609	CA	VAL	181	4.140 -97.857 116.119 1.00 35.27 B	C
	MOTA	2610	CB	VAL	181	4.265 -97.083 117.441 1.00 35.75 B	C
	ATOM	2611	CG1		181	2.911 -96.993 118.104 1.00 36.59 B	C
10	MOTA	2612	CG2	VAL	181	5.258 -97.782 118.362 1.00 36.26 B	C
	ATOM	2613	С	VAL	181	3.148 -97.131 115.220 1.00 35.36 B	C
	MOTA	2614	0	VAL	181	1.986 -97.515 115.151 1.00 35.38 B	0
	MOTA	2615	N	PHE	182	3.599 -96.079 114.538 1.00 35.49 B	N
	ATOM	2616	CA	PHE	182	2.726 -95.330 113.630 1.00 35.30 B	C
15	MOTA	2617	CB	PHE	182	3.431 -94.071 113.117 1.00 33.92 B	C
	ATOM	2618	CG	PHE	182	2.597 -93.254 112.164 1.00 32.96 B	C
	MOTA	2619	CD1	PHE	182	1.647 -92.359 112.640 1.00 32.81 B	C
	MOTA	2620	CD2	PHE	182	2.760 -93.386 110.786 1.00 32.65 B	C
	MOTA	2621	CE1	PHE	182	0.871 -91.604 111.759 1.00 32.61 B	C
20	ATOM	2622	CE2	PHE	182	1.993 -92.640 109.897 1.00 32.30 B	C
	ATOM	2623	CZ	PHE	182	1.047 -91.746 110.382 1.00 32.70 B	C
	MOTA	2624	С	PHE	182	2.349 -96.212 112.439 1.00 36.18 B	C
	ATOM	2625	Ō	PHE	182	1.212 -96.183 111.966 1.00 35.72 B	O
	ATOM	2626	N	ARG	183	3.315 -96.990 111.958 1.00 37.31 B	N
25	ATOM	2627	CA	ARG	183	3.098 -97.885 110.830 1.00 39.17 B	C
	ATOM	2628	СВ	ARG	183	4.427 -98.506 110.383 1.00 39.31 B	Č
	ATOM	2629	CG	ARG	183	5.192 -97.668 109.381 1.00 39.52 B	Č
	ATOM	2630	CD	ARG	183	6.380 -98.428 108.809 1.00 41.16 B	
	ATOM	2631	NE	ARG	183	7.596 -98.227 109.593 1.00 43.06 B	
30	ATOM	2632	CZ	ARG	183	8.263 -99.187 110.224 1.00 43.53 B	
•••	ATOM	2633	NH1		183	7.840-100.445 110.179 1.00 43.79 B	
	ATOM	2634	NH2		183	9.370 -98.885 110.892 1.00 43.85 B	
	ATOM	2635	С	ARG	183	2.094 -99.003 111.108 1.00 39.98 B	
	ATOM	2636	ō	ARG	183	1.442 -99.493 110.187 1.00 39.52 B	
35	ATOM	2637	N	SER	184	1.962 -99.398 112.372 1.00 41.05 B	
•••	ATOM	2638	CA	SER	184	1.054-100.481 112.735 1.00 42.09 B	
	ATOM	2639	СВ	SER	184	1.462-101.079 114.083 1.00 42.35 B	
	ATOM	2640	OG	SER	184	1.270-100.153 115.138 1.00 44.21 B	
	ATOM	2641	C	SER	184	-0.434-100.137 112.765 1.00 42.40 B	
40	ATOM	2642	Ö	SER	184	-1.263-101.034 112.899 1.00 42.68 B	
••	ATOM	2643	N	LEU	185	-0.788 -98.860 112.648 1.00 42.68 B	
	ATOM	2644	CA	LEU	185	-2.201 -98.499 112.660 1.00 42.79 E	
	ATOM	2645	CB	LEU	185	-2.441 -97.131 113.330 1.00 43.53 E	
	ATOM	2646	CG	LEU	185	-1.421 -96.007 113.534 1.00 44.02 E	
45	ATOM	2647		. LEU	185	-2.140 -94.742 113.988 1.00 43.73 E	
10	ATOM	2648		LEU	185	-0.417 -96.404 114.589 1.00 44.56 E	
	ATOM	2649	C	LEU	185	-2.831 -98.510 111.271 1.00 42.68 E	
	ATOM	2650	Ö	LEU	185	-2.133 -98.457 110.258 1.00 42.19 E	
	ATOM	2651	N	PRO	186	-4.171 -98.598 111.209 1.00 42.84 E	
50	MOTA	2652	CD	PRO	186	-5.129 -98.602 112.327 1.00 42.91 E	
00	MOTA	2653	CA	PRO	186	-4.877 -98.615 109.926 1.00 43.29 E	
	ATOM	2654	CB	PRO	186	-6.351 -98.617 110.337 1.00 43.26 E	
		2655	CG	PRO	186	-6.338 -97.972 111.696 1.00 43.70 E	
	ATOM	2656	C	PRO	186	-4.512 -97.421 109.054 1.00 43.49 E	
55	ATOM		0	PRO	186	-4.262 -96.326 109.556 1.00 43.14 B	
	ATOM	2657				-4.282 -96.326 109.336 1.00 43.14 E	
	MOTA	2658			187	-4.137 -96.613 106.784 1.00 43.56 F	
	MOTA	2659		ILE	187		
	MOTA	2660	CB	ILE	187	-4.406 -97.082 105.337 1.00 43.82 H	3 C

-215-

	MOTA	2661	CG2		187	-3.939	-96.018	104.353	1.00 43.79	В	С
	MOTA	2662	CG1	ILE	187	-3.667	-98.395	105.063	1.00 44.06	В	С
	MOTA	2663	CD1		187	-2.156	-98.288	105.188	1.00 44.66	В	C
_	MOTA	2664	С	ILE	187		-95.325		1.00 43.43	В	C
5	MOTA	2665		ILE	187		-94.232		1.00 42.67	В	0
	MOTA	2666	N	GLU	188	-6.214	-95.451		1.00 43.55	В	N
	ATOM	2667		GLU	188	-7.039	-94.273	107.496	1.00 44.32	В	C
	MOTA	2668		GLU	188	-8.514	-94.658	107.582	1.00 45.62	В	C
	ATOM	2669	CG	GLU	188	-9.421	-93.446	107.496	1.00 48.84	В	C
10	MOTA	2670	CD	GLU	188	-8.978	-92.471	106.406	1.00 50.12	В	C
	MOTA	2671	OE1	GLU	188	-8.919	-92.875	105.223	1.00 51.29	В	0
	MOTA	2672	OE2	GLU	188	-8.684	-91.302	106.737	1.00 50.87	В	0
	ATOM	2673	С	GLU	188	-6.635	-93.469	108.735	1.00 43.37	В	C
	MOTA	2674	0	GLU	188	-6.760	-92.245	108.748	1.00 43.27	В	0
15	MOTA	2675	N	ASP	189	-6.166	-94.149	109.776	1.00 42.33	В	N
	ATOM	2676	CA	ASP	189	-5.720	-93.457	110.979	1.00 41.76	В	C
	ATOM	2677	CB	ASP	189	-5.510	-94.442	112.134	1.00 42.89	В	C
	ATOM	2678	CG	ASP	189	-6.811	-94.832	112.806	1.00 44.75	В	С
	ATOM	2679	OD1	ASP	189	-6.768	-95.471	113.879	1.00 46.20	В	0
20	MOTA	2680	OD2	ASP	189	-7.882	-94.498	112.258	1.00 45.42	В	0
	MOTA	2681	С	ASP	189			110.683	1.00 40.38	В	C
	MOTA	2682	0	ASP	189			111.102	1.00 40.12	В	O
	ATOM	2683	N	GLN	. 190			109.955	1.00 39.17	В	N
	MOTA	2684	CA	GLN	190			109.592	1.00 38.44	В	C
25	ATOM	2685	CB	GLN	190			108.725	1.00 37.85	В	C
	MOTA	2686	CG	GLN	190			109.373	1.00 38.72	В	Č
	ATOM	2687	CD	GLN	190	-0.103	-95.854	108.560	1.00 38.85	В	Ċ
	ATOM	2688		GLN	190			108.789	1.00 38.95	В	ō
	MOTA	2689	NE2	GLN	190			107.611	1.00 39.18	В	N
30	ATOM	2690	С	GLN	190			108.822	1.00 37.77	В	C
	ATOM	2691	O	GLN	190			109.077	1.00 38.02	В	ō
	ATOM	2692	N	ILE	191			107.877	1.00.37.50	В	N
	ATOM	2693	CA	ILE	191			107.061	1.00 37.36	В	C
	ATOM	2694	СВ	ILE	191			105.964	1.00 38.55	В	Ċ
35	ATOM	2695	CG2	ILE	191			105.059	1.00 38.60	В	C
	ATOM	2696	CG1		191			105.138	1.00 39.51	В	C
	ATOM	2697	CD1	ILE	191			104.353	1.00 41.55	В	C
	ATOM	2698	С	ILE	191			107.919	1.00 36.51	В	C
	ATOM	2699	0	ILE	191			107.804	1.00 36.70	В	0
40	ATOM	2700	N	SER	192	-5.312	-89.606	108.776	1.00 35.03	В	N
	ATOM	2701	CA	SER	192			109.646	1.00 34.26	В	C
	MOTA	2702	СВ	SER	192			110.446	1.00 34.74	В	С
	MOTA	2703	OG	SER	192	-8.107	-89.757	109.586	1.00 35.76	В	0
	MOTA	2704	С	SER	192	-4.982	-87.956	110.608	1.00 32.87	В	C
45	MOTA	2705	0	SER	192			110.853	1.00 31.92	В	0
	MOTA	2706	N	LEU	193			111.160	1.00 31.50	В	N
	MOTA	2707	CA	LEU	193			112.085	1.00 30.70	В	C
	MOTA	2708	СВ	LEU	193			112.786	1.00 29.93	В	C
	MOTA	2709	CG	LEU	193			113.746	1.00 29.73	В	C
50	MOTA	2710		LEU	193			114.450	1.00 29.19	В	C
	ATOM	2711		LEU	193			114.765		В	C
	ATOM	2712	C	LEU	193			3 111.337		В	C
	MOTA	2713	ō	LEU	193			111.789		В	ō
	ATOM	2714	N	LEU	194			110.187		В	N
55	ATOM	2715	CA	LEU	194			109.389		В	C
	ATOM	2716	CB	LEU	194			108.142		В	C
	ATOM	2717		LEU	194			9 107.333		В	
	ATOM	2718		LEU	194			106.557		В	
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-216-

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	MOTA	2719		LEU	194		-87.032		1.00 33.53	В	C
	ATOM	2720	С	LEU	194		-85.589		1.00 32.06	В	C
	MOTA	2721	0	LEU	194		-84.523		1.00 31.90	В	0
_	ATOM	2722	N	LYS	195		-85.651	108.402	1.00 32.21	В	N
5	MOTA	2723	CA	LYS	195			108.014	1.00 32.26	В	C
	MOTA	2724	CB	LYS	195	-4.643	-84.832	107.404	1.00 34.49	В	C
	MOTA	2725	CG	LYS	195	-4.562	-85.427	106.005	1.00 36.99	В	C
	MOTA	2726	CD	LYS	195	-5.851	-86.146	105.619	1.00 38.55	В	C
	MOTA	2727	CE	LYS	195		-85.223	105.632	1.00 39.77	В	C
10	MOTA	2728	NZ	LYS	195		-85.939	105.131	1.00 41.50	В	N
	ATOM	2729	C	LYS	195		-83.517		1.00 31.45	В	C
	ATOM	2730	ŏ	LYS	195		-82.292	109.079	1.00 30.78	В	ŏ
	ATOM	2731	N	GLY	196			110.339	1.00 29.85	В	N
	ATOM	2732	CA	GLY	196		-83.303	111.509	1.00 28.37	В	C
15	ATOM	2733	C	GLY	196			112.195	1.00 26.84		C
.0	ATOM	2734	o	GLY	196		-81.621	112.195		В	
									1.00 26.88	В	0
	ATOM	2735	N	ALA	197			112.085	1.00 25.28	В	N
	ATOM	2736	CA	ALA	197			112.785	1.00 23.92	В	C
20	ATOM	2737	СВ	ALA	197			113.816	1.00 23.40	В	C
20	ATOM	2738	C	ALA	197			111.978	1.00 22.01	В	С
	MOTA	2739	0	ALA	197			112.550	1.00 20.56	В	0
	MOTA	2740	N	ALA	198			110.668	1.00 20.97	В	N
	ATOM	2741	CA	ALA	198	1.737	-82.073	109.836	1.00 20.46	В	C
	MOTA	2742	CB	ALA	198	1.406	-82.284	108.349	1.00 20.75	В	C
25	MOTA	2743	C	ALA	198	2.188	-80.631	110.071	1.00 19.62	В	C
	ATOM	2744	0	ALA	198	3.359	-80.381	110.365	1.00 19.14	В	0
	MOTA	2745	N	VAL	199	1.262	-79.689	109.935	1.00 19.02	В	N
	ATOM	2746	CA	VAL	199	1.566	-78.276	110.125	1.00 19.01	В	C
	ATOM	2747	CB	VAL	199	0.365	-77.401	109.738	1.00 19.49	В	C
30	ATOM	2748		VAL	199			110.073	1.00 18.87	В	Č
	ATOM	2749		VAL	199			108.243	1.00 19.44	В	Č.
	ATOM	2750	c	VAL	199			111.555	1.00 18.82	В	Ċ.
	ATOM	2751	ŏ	VAL	199			111.766	1.00 19.08	В	ŏ
	MOTA	2752	N	GLU	200			112.531	1.00 17.97	В	N
35	ATOM	2753	CA	GLU	200			113.934	1.00 17.37	В	C
00	MOTA	2754	CB	GLU	200			114.850	1.00 18.45	В	
	ATOM	2755	CG	GLU	200			115.030	1.00 10.13		C
										В	
	ATOM	2756	CD	GLU	200			115.866	1.00 21.56	В	C
40	MOTA	2757	OE1		200			116.765	1.00 21.43	В	0
40	MOTA	2758	OE2		200		-79.197		1.00 22.35	В	0
	MOTA	2759	C	GLU	200	3.138		114.202	1.00 17.94	В	C
	MOTA	2760	0	GLU	200			114.830	1.00 18.17	В	0
	MOTA	2761	N	ILE	201			113.716	1.00 17.97	В	N
4 ==	ATOM	2762	CA	ILE	201			113.897	1.00 17.91	В	С
45	MOTA	2763	CB	ILE	201			113.335	1.00 18.26	В	С
	MOTA	2764	CG2		201			2 113.260	1.00 17.92	В	С
	ATOM	2765		LILE	201			114.233	1.00 17.28	В	C
	MOTA	2766	CD1	ILE	201	3.815	-84.368	3 113.701	1.00 18.61	В	C
	MOTA	2767	C	ILE	201	5.869	-79.731	113.255	1.00 17.32	В	C
50	MOTA	2768	0	ILE	201	6.953	-79.547	7 113.815	1.00 18.72	В	0
	ATOM	2769	N	CYS	202	5.567	-79.165	112.095	1.00 16.54	В	N
	MOTA	2770		CYS	202			2 111.434	1.00 16.29	В	C
	ATOM	2771	СВ	CYS	202			110.062	1.00 16.39	В	Č
	ATOM	2772	SG	CYS	202			108.838	1.00 16.45	В	S
55	ATOM	2773		CYS	202			9 112.295	1.00 15.32	В	C
	ATOM	2774		CYS	202			112.293	1.00 13.32	В	0
					202			3 112.386 3 112.924			
	MOTA	2775		HIS						В	
	MOTA	2776	CA	HIS	203	0.061	-/5.29	0 113.768	1.00 15.80	В	С

-217-

	MOTA	2777		HIS	203	4.750 -74.610		1.00 15.84	В	С
	MOTA	2778		HIS	203	4.173 -73.757		1.00 15.00	В	C
	MOTA	2779	CD2		203	3.148 -73.977		1.00 15.47	В	С
_	MOTA	2780	ND1		203	4.719 -72.545		1.00 15.56	В	N
5	MOTA	2781	CE1		203	4.058 -72.056		1.00 15.06	В	С
	MOTA	2782		HIS	203	3.100 -72.906		1.00 15.27	В	N
	MOTA	2783		HIS	203	6.886 -75.646		1.00 15.74	В	С
	MOTA	2784	0	HIS	203	7.738 -74.867		1.00 16.61	В	0
40	MOTA	2785	N	ILE	204	6.643 -76.818		1.00 14.51	В	N
10	MOTA	2786	CA	ILE	204	7.421 -77.263		1.00 15.77	В	C
	MOTA	2787	CB	ILE	204	6.914 -78.643		1.00 14.78	В	С
	MOTA	2788			204	7.885 -79.192		1.00 14.01	В	C
	MOTA	2789	CG1		204	5.496 -78.495		1.00 14.35	В	С
4-	MOTA	2790		ILE	204	4.849 -79.812		1.00 11.99	В	С
15	MOTA	2791	С	ILE	204	8.890 -77.404		1.00 15.99	В	С
	MOTA	2792	0	ILE	204	9.803 -76.963		1.00 14.96	В	0
	MOTA	2793	N	VAL	205	9.108 -78.011		1.00 16.33	В	N
	MOTA	2794	CA	VAL	205	10.463 -78.208		1.00 18.21	В	С
	MOTA	2795	CB	VAL	205	10.455 -79.139		1.00 17.84	В	С
20	ATOM	2796	CG1		205	11.796 -79.058		1.00 17.90	В	C
	MOTA	2797		VAL	205	10.169 - 80.569		1.00 18.55	В	С
	MOTA	2798	С	VAL	205	11.153 -76.90		1.00 17.83	В	С
	MOTA	2799	0	VAL	205	12.317 -76.698		1.00 17.35	В	0
	ATOM	2800	N	LEU	206	10.434 -76.02		1.00 18.27	В	N
25	MOTA	2801	CA	LEU	206	11.006 -74.74		1.00 19.32	В	С
	MOTA	2802	CB	LEU	206	10.051 -74.03		1.00 19.42	В	C
	MOTA	2803	CG	LEU	206	10.452 -73.90		1.00 21.56	В	C
	MOTA	2804		LEU	206	11.505 -74.93		1.00 21.35	В	C
	MOTA	2805		LEU	206	9.196 -74.03		1.00 21.44	В	С
30	MOTA	2806	C	LEU	206	11.318 -73.82		1.00 18.20	В	С
	ATOM	2807	0	LEU	206	12.121 -72.90		1.00 17.70	В	0
	ATOM	2808	N	ASN	207	10.688 -74.07		1.00 17.51	В	N
	ATOM	2809	CA	ASN	207	10.918 -73.25		1.00 17.40	В	С
25	ATOM	2810	CB	ASN	207	10.124 -73.77		1.00 15.99	В	С
35	ATOM	2811	CG	ASN	207	10.184 -72.82		1.00 16.60	В	C
	ATOM	2812		ASN	207	10.860 -73.10		1.00 15.13	В	0
	MOTA	2813		ASN	207	9.485 -71.70		1.00 13.67	В	N
	MOTA	2814	C	ASN	207	12.387 -73.14		1.00 18.07	В	C
40	MOTA	2815	0	ASN	207	12.804 -72.13		1.00 17.57	В	0
40	MOTA	2816	N	THR	208	13.172 -74.17		1.00 18.22	В	N
	MOTA	2817	CA	THR	208	14.595 -74.14		1.00 20.72	В	C
	ATOM	2818	СВ	THR	208	15.258 -75.53			В	
	ATOM	2819		THR	208	15.018 -76.01		1.00 23.70	В	0
AE	MOTA	2820		THR	208	14.676 -76.54		1.00 22.78	В	C
45	ATOM	2821	C	THR	208	15.366 -73.10		1.00 20.46	В	C
	MOTA	2822	0	THR	208	16.501 -72.78		1.00 21.62	В	0
	MOTA	2823	N	THR	209	14.760 -72.56		1.00 19.69	В	N
	MOTA	2824	CA	THR	209	15.423 -71.53		1.00 19.16	В	C
50	MOTA	2825	CB	THR	209	15.153 -71.70		1.00 18.90	В	C
50	ATOM	2826		THR	209	13.776 -71.40		1.00 17.30	В	0
	ATOM	2827	CG2		209	15.474 -73.12		1.00 18.39	В	C
	ATOM	2828	C	THR	209	14.944 -70.13			В	C
	ATOM	2829		THR	209	15.456 -69.14			В	0
E E	ATOM	2830		PHE	210	13.962 -70.05			В	
55	ATOM	2831	CA	PHE	210	13.429 -68.76			В	C
	ATOM	2832		PHE	210	12.107 -68.93			В	C
	ATOM	2833		PHE	210	11.307 -67.66			В	_
	MOTA	2834	CD1	. PHE	210	10.694 -67.08	115.914	1.00 18.35	В	С

-218-

			_				
	MOTA	2835	CD2		210	11.161 -67.046 118.263 1.00 19.05 B C	
	MOTA	2836	CE1		210	9.945 -65.909 116.039 1.00 18.54 B C	
	MOTA	2837		PHE	210	10.409 -65.865 118.401 1.00 19.42 B C	
_	MOTA	2838	CZ	PHE	210	9.802 -65.299 117.286 1.00 18.58 B C	
5	MOTA	2839	C	PHE	210	14.411 -68.002 116.986 1.00 20.77 B C	
	ATOM	2840	0	PHE	210	14.847 -68.498 118.021 1.00 20.70 B O	
	MOTA	2841		CYS	211	14.759 -66.794 116.565 1.00 22.21 B N	
	ATOM	2842	CA	CYS	211	15.674 -65.953 117.327 1.00 24.26 B C	
40	ATOM	2843	CB	CYS	211	16.575 -65.155 116.391 1.00 24.98 B C	
10	ATOM	2844	SG	CYS	211	17.664 -64.026 117.267 1.00 27.94 B S	
	MOTA	2845	C	CYS	211	14.824 -64.996 118.148 1.00 25.17 B C	
	MOTA	2846	0	CYS	211	14.060 -64.209 117.586 1.00 24.50 B O	
	MOTA	2847	N	LEU	212	14.950 -65.076 119.471 1.00 25.78 B N	
15	MOTA	2848	CA	LEU	212	14.173 -64.229 120.375 1.00 27.77 B C	
15	MOTA	2849	CB	LEU	212	14.396 -64.652 121.830 1.00 26.74 B C	
	MOTA	2850	CG	LEU	212	13.735 -65.968 122.237 1.00 26.59 B C	
	MOTA	2851	CD1	-	212	14.046 -66.279 123.700 1.00 26.25 B C	
	MOTA	2852	CD2		212	12.235 -65.863 122.014 1.00 24.89 B C 14.448 -62.739 120.253 1.00 28.72 B C	
20	MOTA	2853	C	LEU	212		
20	ATOM	2854	0	LEU	212	13.521 -61.931 120.271 1.00 29.38 B O	
	ATOM	2855	N	GLN	213	15.720 -62.379 120.140 1.00 30.42 B N	
	ATOM	2856	CA	GLN	213	16.108 -60.982 120.027 1.00 32.34 B C	
	MOTA	2857	CB	GLN	213	17.631 -60.869 119.893 1.00 35.12 B C 18.122 -59.462 119.576 1.00 38.96 B C	
25	MOTA	2858	CG CD	GLN	213		
25	ATOM	2859		GLN	213		
	ATOM	2860 2861	NE2	GLN GLN	213 213	19.566 -58.754 121.357 1.00 42.98 B O 17.500 -57.858 121.284 1.00 42.35 B N	
	ATOM ATOM	2862	C	GLN	213	15.453 -60.262 118.846 1.00 32.03 B C	
	ATOM	2863	0	GLN	213	15.005 -59.126 118.986 1.00 32.80 B O	
30	ATOM	2864	Ŋ	THR	214	15.390 -60.919 117.691 1.00 30.84 B N	
30	ATOM	2865	CA	THR	214	14.828 -60.288 116.497 1.00 29.82 B C	
	ATOM	2866	CB	THR	214	15.808 -60.393 115.316 1.00 29.30 B C	
	ATOM	2867	OG1		214	16.083 -61.773 115.049 1.00 28.95 B	
	ATOM	2868	CG2		214	17.108 -59.679 115.636 1.00 30.14 B C	
35	MOTA	2869	C	THR	214	13.472 -60.792 116.009 1.00 29.36 B	
00	ATOM	2870	Ö	THR	214	12.941 -60.264 115.032 1.00 28.67 B	
	ATOM	2871	N	GLN	215	12.918 -61.805 116.670 1.00 28.97 B N	
	ATOM	2872	CA	GLN	215	11.623 -62.361 116.273 1.00 29.50 B	
	ATOM	2873	СВ	GLN	215	10.533 -61.284 116.375 1.00 30.88 B	
40	ATOM	2874	CG	GLN	215	10.336 -60.704 117.764 1.00 33.91 B	
	MOTA	2875	CD	GLN	215	9.754 -61.711 118.726 1.00 35.71 B C	
	ATOM	2876		GLN	215	8.651 -62.221 118.513 1.00 37.61 B	
	ATOM	2877		GLN	215	10.492 -62.010 119.793 1.00 36.76 B N	
	ATOM	2878	C	GLN	215	11.670 -62.890 114.834 1.00 28.46 B C	
45	ATOM	2879	ŏ	GLN	215	10.696 -62.774 114.093 1.00 28.52 B	
	ATOM	2880	N	ASN	216	12.801 -63.465 114.442 1.00 26.98 B	
	ATOM	2881	CA	ASN	216	12.960 -63.990 113.092 1.00 25.74 B	
	ATOM	2882	CB	ASN	216	14.085 -63.250 112.363 1.00 27.52 B	
	ATOM	2883	CG	ASN	216	13.770 -61.786 112.093 1.00 28.70 B	2
50	ATOM	2884		ASN	216	14.664 -61.022 111.749 1.00 27.69 B	
	ATOM	2885		ASN	216	12.503 -61.394 112.228 1.00 29.92 B	
	ATOM	2886	C	ASN	216		2
	ATOM	2887	ō	ASN	216		0
	ATOM	2888	N	PHE	217		N
55	ATOM	2889	CA	PHE	217		C
	ATOM	2890	СВ	PHE	217		С
	ATOM	2891	CG	PHE	217		С
	ATOM	2892		PHE	217		С

-219-

	MOTA	2893	CD2		217			112.733	1.00 19.92	В	C
	MOTA	2894		PHE	217			112.664	1.00 18.54	В	C
	MOTA	2895		PHE	217			113.453	1.00 19.66	В	C
_	MOTA	2896	CZ	PHE	217			113.415	1.00 19.48	В	C
5	MOTA	2897	С	PHE	217			111.057	1.00 22.98	В	С
	MOTA	2898	0	PHE	217			109.895	1.00 21.70	В	0
	MOTA	2899	N	LEU	218			111.645	1.00 23.53	В	N
	MOTA	2900	CA	LEU	218			110.957	1.00 24.87	В	C
40	MOTA	2901	CB	LEU	218			111.930	1.00 26.08	В	C
10	MOTA	2902	CG	LEU	218			112.436	1.00 27.99	В	С
	MOTA	2903	CD1		218			113.126	1.00 27.86	В	С
	MOTA	2904	CD2		218			113.413	1.00 27.96	В	C
	ATOM	2905	С	LEU	218			110.383	1.00 25.07	В	С
4.5	MOTA	2906	0	LEU	218			111.115	1.00 25.64	В	0
15	MOTA	2907	N	CYS	219			109.069	1.00 24.23	В	N
	MOTA	2908	CA	CYS	219			108.396	1.00 23.85	В	C
	MOTA	2909	CB	CYS	219	15:935	-71.263	107.674	1.00 22.48	В	С
	MOTA	2910	SG	CYS	219	14.462	-71.225	108.747	1.00 19.92	В	S
	MOTA	2911	C	CYS	219	18.406	-70.868	107.398	1.00 24.42	В	С
20	MOTA	2912	0	CYS	219	18.231	-70.505	106.227	1.00 22.82	В	0
	MOTA	2913	N	GLY	220	19.590	-71.252	107.870	1.00 25.23	В	N
	MOTA	2914	CA	GLY	220	20.764	-71.214	107.021	1.00 24.90	В	С
	MOTA	2915	C	GLY	220	20.996	-69.754	106.695	1.00 24.77	В	C
	MOTA	2916	0	GLY	220	21.031	-68.922	107.601	1.00 24.69	В	0
25	MOTA	2917	N	PRO	221	21.152	-69.401	105.412	1.00 24.50	В	N
	MOTA	2918	CD	PRO	221	21.305	-70.265	104.229	1.00 23.93	В	C
	MOTA	2919	CA	PRO	221	21.374	-67.993	105.060	1.00 24.42	В	С
	MOTA	2920	CB	PRO	221	22.053	-68.090	103.699	1.00 23.72	В	С
	MOTA	2921	CG	PRO	221	21.356	-69.247	103.085	1.00 23.75	В	С
30	ATOM	2922	С	PRO	221	20.073	-67.181	104.995	1.00 23.85	В	C
	MOTA	2923	0	PRO	221	20.108	-65.967	104.811	1.00 23.61	В	0
	MOTA	2924	N	LEU	222	18.935	-67.858	105.153	1.00 22.94	В	N
	MOTA	2925	CA	LEU	222	17.627	-67.209	105.084	1.00 22.55	В	C
	MOTA	2926	СВ	LEU	222	16.595	-68.162	104.478	1.00 20.79	В	C
35	MOTA	2927	CG	LEU	222	16.913	-68.732	103.100	1.00 19.76	В	C
	MOTA	2928	CD1	LEU	222	15.742	-69.560	102.623	1.00 20.37	В	C
	MOTA	2929	CD2	LEU	222	17.199	-67.594	102.122	1.00 20.15	В	C
	MOTA	2930	C	LEU	222	17.093	-66.695	106.415	1.00 22.84	В	C
	MOTA	2931	0	LEU	222	17.341	-67.275	107.473	1.00 23.24	В	0
40	MOTA	2932	N	ARG	223			106.333	1.00 22.89	В	N
	MOTA	2933	CA	ARG	223	15.733	-64.960	107.485	1.00 24.01	В	C
	MOTA	2934	CB	ARG	223			107.782	1.00 26.47	В	C
	MOTA	2935	CG	ARG	223			108.768	1.00 31.77	В	C
	MOTA	2936	CD	ARG	223			108.616	1.00 35.27	В	C
45	ATOM	2937	NE	ARG	223			107.349	1.00 38.31	В	N
	ATOM	2938	CZ	ARG	223	16.314	-59.714	106.740	1.00 39.39	В	C
	MOTA	2939		ARG	223			107.279	1.00 41.22	В	N
	ATOM	2940		ARG	223			105.600	1.00 40.79	В	N
	ATOM	2941	С	ARG	223	14.265	-64.663	107.183	1.00 23.59	В	С
50	MOTA	2942	0	ARG	223			106.287	1.00 22.38	В	0
	MOTA	2943	N	TYR	224			107.930	1.00 22.01	В	N
	MOTA	2944	CA	TYR	224			107.742	1.00 21.48	В	С
	MOTA	2945	СВ	TYR	224			107.718	1.00 20.04	В	С
	MOTA	2946	CG	TYR	224			106.615	1.00 19.13	В	С
55	MOTA	2947		TYR	224			106.851	1.00 17.91	В	C
	MOTA	2948		TYR	224			105.848	1.00 18.05	В	C
	MOTA	2949		TYR	224			105.338	1.00 17.45	В	C
	ATOM	2950	CE2	TYR	224	11.392	-68.124	104.319	1.00 17.93	В	C

-220-

	MOTA	2951	CZ	TYR	224	12.328	-69.118	104.587	1.00 17.71		C
	MOTA	2952	OH	TYR	224	12.714	-69.995	103.606	1.00 17.71		0
	MOTA	2953	С	TYR	224	11.352	-64.239	108.872	1.00 21.91	В	C
	MOTA	2954	0	TYR	224	11.619	-64.502	110.043	1.00 21.72		0
5	MOTA	2955	N	THR	225	10.556	-63.238	108.509	1.00 21.54		N
	ATOM	2956	CA	THR	225	9.942	-62.340	109.478	1.00 21.65		C
	MOTA	2957	СВ	THR	225	10.335	-60.874	109.202	1.00 23.19		C
	MOTA	2958	OG1	THR	225	9.847	-60.492	107.912	1.00 22.96	В	0
	ATOM	2959	CG2	THR	225	11.853	-60.695	109.232	1.00 23.33	В	C
10	ATOM	2960	С	THR	225	8.418	-62.421	109.416	1.00 20.84	В	С
	ATOM	2961	0	THR	225	7.849	-63.042	108.513	1.00 19.99	В	0
	ATOM	2962	N	ILE	226	7.764	-61.773	110.376	1.00 19.42	В	N
	ATOM	2963	CA	ILE	226	6.311	-61.746	110.430	1.00 18.00	В	С
	ATOM	2964	СВ	ILE	226	5.837	-61.101	111.768	1.00 17.71	В	С
15	ATOM	2965	CG2	ILE	226		-59.625		1.00 16.28	В	С
•••	ATOM	2966	CG1	ILE	226		-61.306		1.00 15.92	В	C
	ATOM	2967	CD1	ILE	226		-60.925		1.00 13.01	В	С
	ATOM	2968	C	ILE	226		-60.988		1.00 18.53	В	C
	ATOM	2969	ŏ	ILE	226			108.754	1.00 17.76	В	Ō
20	ATOM	2970	N	GLU	227			108.649	1.00 18.32	В	N
20	ATOM	2971	CA	GLU	227			107.468	1.00 19.11	В	c
	ATOM	2972	СВ	GLU	227			107.103	1.00 20.59	В	Ċ
	ATOM	2973	CG	GLU	227			107.959	1.00 20.58	В	Č
	ATOM	2974	CD	GLU	227			109.396	1.00 21.61	В	č
25	ATOM	2975		GLU	227			109.617	1.00 23.10	В	ŏ
20	ATOM	2976	OE2		227			110.308	1.00 22.37	В	ŏ
	ATOM	2977	C	GLU	227			106.273	1.00 18.86	В	Č
		2978	0	GLU	227			105.416	1.00 18.23	В	ŏ
	MOTA				228			106.199	1.00 18.23	В	N
30	MOTA	2979	N	ASP	228			105.133	1.00 18.69	В	C
30	ATOM	2980	CA	ASP					1.00 18.03	В	c
	ATOM	2981	CB	ASP	228			105.088	1.00 18.93		C
	MOTA	2982	CG	ASP	228			104.950	1.00 19.98	В	0
	ATOM	2983		ASP	228			104.031		В	
25	ATOM	2984		ASP	228			105.754	1.00 19.87	В	0
35	MOTA	2985	C	ASP	228			105.102	1.00 18.01	В	C
	MOTA	2986	0	ASP	228			104.064	1.00 18.44	В	0
	MOTA	2987	N	GLY	229			106.289	1.00 17.20	В	N
	MOTA	2988	CA	GLY	229			106.392	1.00 17.52	В	C
40	ATOM	2989	C	GLY	229			106.035	1.00 17.70	В	C
40	ATOM	2990	0	GLY	229			105.330	1.00 18.08	В	0
	MOTA	2991	N	ALA	230			106.510	1.00 17.31	В	N
	MOTA	2992	CA	ALA	230			106.237	1.00 17.67	В	C
	MOTA	2993	CB	ALA	230			107.031	1.00 17.60	В	C
4.5	MOTA	2994	С	ALA	230			104.749	1.00 18.51	В	C
45	MOTA	2995	0	ALA	230			104.231	1.00 17.21	В	0
	MOTA	2996		ARG	231			104.060	1.00 19.86	В	N
	MOTA	2997		ARG	231			102.643	1.00 20.24	В	С
	MOTA	2998		ARG	231			102.173	1.00 21.54	В	C
	MOTA	2999	CG	ARG	231			2 102.843	1.00 23.12	В	C
50	MOTA	3000	CD	ARG	231			5 102.506	1.00 23.94	В	C
	MOTA	3001		ARG	231			5 101.092	1.00 25.20	В	N
	MOTA	3002		ARG	231			5 100.553	1.00 25.86	В	С
	MOTA	3003	NH	l ARG	231			1 101.301		В	N
	ATOM	3004	NH	2 ARG	231		1 -55.74			В	N
55	ATOM	3005		ARG	231			9 101.765		В	С
	MOTA	3006		ARG	231	1.561	L -60.63	2 100.640	1.00 19.52		_
	MOTA	3007		VAL	232	1.865	-62.15	3 102.256		В	N
	ATOM	3008		VAL	232	1.239	-63.19	5 101.450	1.00 19.34	В	С

-221-

	MOTA	3009	СВ	VAL	232	1.927	-64.592	101.612	1.00 20.66	В	С
	MOTA	3010	CG1		232			101.307	1.00 19.33	В	C
	MOTA	3011		VAL	232	1.671	-65.169	103.017	1.00 18.79	В	C
_	MOTA	3012	С	VAL	232	-0.245	-63.330	101.779	1.00 19.07	В	C
5	MOTA	3013	0	VAL	232			101.230	1.00 17.55	В	0
	ATOM	3014	N	GLY	233			102.680	1.00 19.78	В	N
	MOTA	3015	CA	GLY	233			103.008	1.00 20.41	В	С
	MOTA	3016	C	GLY	233	-2.643	-62.915	104.397	1.00 21.13	В	C
40	MOTA	3017	0	GLY	233			104.719	1.00 21.49	В	0
10	MOTA	3018	N	PHE	234	-1.806	-63.541	105.223	1.00 20.51	В	N
	ATOM	3019	CA	PHE	234			106.563	1.00 20.56	В	С
	MOTA	3020	CB	PHE	234	-1.205	-64.706	107.326	1.00 20.73	В	C
	ATOM	3021	CG	PHE	234			106.810	1.00 20.24	В	C
45	MOTA	3022	CD1		234			106.135	1.00 19.02	В	C
15	ATOM	3023	CD2		234			107.035	1.00 19.67	В	С
	MOTA	3024	CE1		234			105.695	1.00 19.63	В	С
	MOTA	3025	CE2	PHE	234			106.597	1.00 19.47	В	С
	MOTA	3026	CZ	PHE	234			105.928	1.00 18.87	В	C
00	MOTA	3027	С	PHE	234			107.362	1.00 20.67	В	C
20	MOTA	3028	0	PHE	234			107.234	1.00 20.71	В	0
	MOTA	3029	N	GLN	235			108.194	1.00 21.02	В	N
	ATOM	3030	CA	GLN	235			109.020	1.00 22.09	В	C
	MOTA	3031	CB	GLN	235			109.548	1.00 22.57	В	C
05	MOTA	3032	CG	GLN	235			108.428	1.00 24.45	В	С
25	MOTA	3033	CD	GLN	235			108.926	1.00 27.02	В	C
	ATOM	3034		GLN	235			109.748	1.00 27.06	В	0
	MOTA	3035	NE2		235			108.423	1.00 27.49	В	N
	ATOM	3036	С	GLN	235			110.173	1.00 21.61	В	С
20	MOTA	3037	0	GLN	235			110.718	1.00 21.23	В	0
30	MOTA	3038	N	VAL	236			110.542	1.00 21.74	В	N
	MOTA	3039	CA	VAL	236			111.616	1.00 22.27	В	C
	ATOM	3040	СВ	VAL	236			111.810	1.00 22.19	В	C
	ATOM	3041		VAL	236			113.032	1.00 22.00	В	С
25	MOTA	3042		VAL	236			110.562	1.00 21.53	В	C
35	ATOM	3043	С	VAL	236			112.944	1.00 22.51	В	C
	ATOM	3044	0	VAL	236			113.604	1.00 22.18	В	0
	ATOM	3045	N	GLU	237			113.332	1.00 22.41	В	N
	ATOM	3046	CA	GLU	237			114.586	1.00 22.96	В	C
40	MOTA	3047	CB	GLU	237			114.748	1.00 25.41	В	C
40	ATOM	3048	CG	GLU	237			115.905	1.00 29.15	В	C
	ATOM	3049	CD	GLU	237			116.076	1.00 31.86	В	C
	MOTA	3050		GLU	237			115.062		В	
	MOTA	3051 3052		GLU	237			117.227	1.00 32.72	В	0
45	MOTA		C	GLU	237			114.628	1.00 21.89	В	C
70	MOTA MOTA	3053 3054	0	GLU	237 238			115.643 113.516	1.00 20.82	В	0
	ATOM		N	PHE	238			113.316	1.00 20.52	В	Ŋ
		3055	CA	PHE				112.033	1.00 19.64 1.00 18.50	В	C
	MOTA MOTA	3056 3057	CB CG	PHE PHE	238 238			3 111.679		В	C
50	ATOM	3058		PHE	238			112.303	1.00 18.24 1.00 18.18	B B	C
00	MOTA	3059	CD2		238			112.303	1.00 18.18	В	C
	ATOM			PHE	238			111.724			
	ATOM	3060 3061	CE1		238			111.983	1.00 18.90 1.00 18.97	B B	C
	ATOM	3062	CEZ	PHE	238			2 111.025	1.00 18.97	В	C
55	ATOM	3062	C	PHE	238			l 113.526	1.00 19.52	В	С
-	ATOM	3064	0	PHE	238			3 114.276	1.00 19.52	В	0
	ATOM	3065	N	LEU	239			7 112.799	1.00 17.83	В	N
	ATOM	3066	CA	LEU	239			3 112.799	1.00 19.31	В	
	ATOM	3000	CA	neo	233	V.3/2	03.303	, 112.040	1.00 21.27	0	C

-222-

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	MOTA	3067		LEU	239	0.881 -62.786 111.918 1.00 19.88 B	
	ATOM	3068		LEU	239	1.358 -63.090 110.485 1.00 21.98 B 0.983 -64.488 110.062 1.00 19.74 B 0	
	ATOM	3069	CD1	-	239 239		Š
5	MOTA	3070 3071	CD2	LEU	239		Š
•	ATOM ATOM	3072		LEU	239		Š
	ATOM	3072		GLU	240		N
	ATOM	3074		GLU	240		C
	ATOM	3075		GLU	240		C
10	ATOM	3076		GLU	240		Ċ
	ATOM	3077		GLU	240		С
	ATOM	3078		GLU	240		0
	ATOM	3079	OE2	GLU	240	1.743 -58.604 115.417 1.00 36.81 B	0
	MOTA	3080	С	GLU	240	0.511 -63.689 117.254 1.00 23.48 B	С
15	MOTA	3081	0	GLU	240		0
	MOTA	3082	N	LEU	241		N
	MOTA	3083	CA	LEU	241		С
	MOTA	3084		LEU	241		C
20	MOTA	3085	CG	LEU	241		C
20	MOTA	3086	CD1		241		C
	MOTA	3087	CD2		241		C
	MOTA	3088	C	LEU	241		C
	ATOM	3089	0	LEU	241		O N
25	MOTA	3090	N	LEU	242	0.666 -66.746 116.265 1.00 19.66 B 1.711 -67.663 115.827 1.00 19.39 B	C
~5	MOTA	3091	CA CB	LEU LEU	242 242	1.711 -67.003 113.827 1.00 13.33 B	c
	ATOM ATOM	3092 3093	CG	LEU	242	2.800 -68.626 113.656 1.00 17.99 B	C
	ATOM	3094		LEU	242	2.679 -70.043 114.206 1.00 17.20 B	č
	ATOM	3095	_	LEU	242	2.593 -68.633 112.148 1.00 17.85 B	č
30	ATOM	3096	C	LEU	242	3.093 -67.301 116.380 1.00 19.08 B	Ċ
	ATOM	3097	ō	LEU	242	3.825 -68.174 116.858 1.00 18.27 B	0
	ATOM	3098	N	PHE	243	3.448 -66.020 116.322 1.00 19.06 B	N
	ATOM	3099	CA	PHE	243	4.746 -65.587 116.820 1.00 20.50 B	C
	MOTA	3100	CB	PHE	243	5.120 -64.209 116.250 1.00 20.80 B	C
35	MOTA	3101	CG	PHE	243	5.719 -64.280 114.866 1.00 21.15 B	С
	MOTA	3102	CD1	PHE	243	4.944 -64.674 113.773 1.00 21.05 B	C
	MOTA	3103	CD2	PHE	243	7.071 -64.015 114.665 1.00 20.91 B	C
	MOTA	3104		PHE	243	5.508 -64.810 112.497 1.00 21.45 B	С
40	MOTA	3105		PHE	243	7.646 -64.149 113.395 1.00 21.14 B	C
40	MOTA	3106	CZ	PHE	243	6.858 -64.549 112.308 1.00 21.10 B	С
	MOTA	3107	С	PHE	243	4.821 -65.589 118.340 1.00 21.66 B	C
	ATOM	3108		PHE	243		•
	ATOM	3109		HIS	244	3.673 -65.424 118.995 1.00 22.31 B 3.612 -65.456 120.448 1.00 23.28 B	C N
45	MOTA	3110 3111		HIS HIS	244 244	2.220 -65.048 120.951 1.00 26.24 B	c
75	MOTA MOTA	3112		HIS	244	1.972 -65.395 122.391 1.00 29.43 B	C
	ATOM	3112		HIS	244	2.047 -64.644 123.516 1.00 30.00 B	č
	ATOM	3114		HIS	244	1.623 -66.666 122.804 1.00 30.79 B	N
	MOTA	3115		HIS	244	1.494 -66.682 124.119 1.00 30.26 B	C
50	ATOM	3116		HIS	244	1.747 -65.469 124.575 1.00 30.77 B	N
_	ATOM	3117		HIS	244	3.904 -66.892 120.857 1.00 21.80 B	С
	ATOM	3118		HIS	244	4.636 -67.133 121.809 1.00 21.67 B	0
	MOTA	3119	N	PHE	245	3.308 -67.837 120.137 1.00 19.90 B	N
	ATOM	3120		PHE	245	3.529 -69.255 120.389 1.00 18.67 B	C
55	MOTA	3121		PHE	245	2.775 -70.104 119.356 1.00 18.04 B	C
	MOTA	3122		PHE	245	3.217 -71.540 119.316 1.00 17.45 B	С
	MOTA	3123		1 PHE	245	2.802 -72.439 120.294 1.00 16.43 B	C
	MOTA	3124	CD	2 PHE	245	4.087 -71.985 118.321 1.00 17.18 B	C

-223-

	MOTA	3125	CE1	PHE	245	3.244	-73.760	120.286	1.00 16.09	В	C
	ATOM	3126	CE2	PHE	245	4.539	-73.306	118.303	1.00 17.01	В	C
	ATOM	3127	CZ	PHE	245		-74.196		1.00 16.45	В	C
_	ATOM	3128	C	PHE	245	5.030	-69.556	120.290	1.00 17.95	В	С
5	MOTA	3129	0	PHE	245	5.600	-70.169	121.183	1.00 17.52	В	0
	ATOM	3130	N	HIS	246	5.666	-69.115	119.206	1.00 16.92	В	N
	ATOM	3131	CA	HIS	246	7.092	-69.365	119.024	1.00 16.61	В	C
	ATOM	3132	CB	HIS	246	7.541	-68.936	117.620	1.00 15.88	В	C
	ATOM	3133	CG	HIS	246	7.208	-69.935	116.554	1.00 16.90	В	C
10	ATOM	3134	CD2	HIS	246	6.248	-69.934	115.599	1.00 17.28	В	С
	ATOM	3135	ND1	HIS	246	7.856	-71.145	116.440	1.00 16.47	В	N
	ATOM	3136	CE1	HIS	246	7.309	-71.848	115.465	1.00 16.06	В	С
	ATOM	3137	NE2	HIS	246	6.330	-71.136	114.940	1.00 15.84	В	N
	ATOM	3138	С	HIS	246	7.959	-68.704	120.095	1.00 16.14	В	C
15	ATOM	3139	0	HIS	246			120.598	1.00 16.15	В	0
	ATOM	3140	N	GLY	247	7.666	-67.461	120.445	1.00 15.88	В	N
	ATOM	3141	CA		247			121.488	1.00 16.58	В	С
	ATOM	3142	C	GLY	247		-67.552	122.820	1.00 17.29	В	С
	ATOM	3143	Ö	GLY	247			123.474	1.00 16.50	В	0
20	ATOM	3144	N	THR	248			123.215	1.00 17.62	В	N
	ATOM	3145	CA	THR	248			124.473	1.00 19.52	В	C
	ATOM	3146	СВ	THR	248			124.715	1.00 20.24	В	Č
	ATOM	3147	OG1		248			124.589	1.00 19.56	В	ŏ
	ATOM	3148	CG2	THR	248			126.110	1.00 20.09	В	Č
25	ATOM	3149	C	THR	248			124.530	1.00 19.85	В	Ċ
	ATOM	3150	ŏ	THR	248			125.519	1.00 18.96	В	ō
	ATOM	3151	N	LEU	249			123.466	1.00 19.93	В	N
	ATOM	3152	CA	LEU	249			123.412	1.00 21.38	В	C
	ATOM	3153	CB	LEU	249			122.145	1.00 21.21	В	Č
30	ATOM	3154	CG	LEU	249			121.875	1.00 19.48	В	Č
-	ATOM	3155		LEU	249			123.015	1.00 21.12	В	Č
	ATOM	3156		LEU	249			120.547	1.00 19.38	В	C
	ATOM	3157	C	LEU	249			123.429	1.00 22.24	В	c
	ATOM	3158	Ö	LEU	249			124.101	1.00 21.93	В	ŏ
35	ATOM	3159	N	ARG	250			122.683	1.00 23.40	В	N
•	ATOM	3160	CA	ARG	250			122.592	1.00 25.09	В	C
	MOTA	3161	CB	ARG	250			121.613	1.00 26.51	В	C
	ATOM	3162	CG	ARG	250			120.465	1.00 28.87	В	Č
	MOTA	3163	CD	ARG	250		-	120.927	1.00 28.96	В	c
40	ATOM	3164	NE	ARG	250		-70.513		1.00 29.63	В	N
40	ATOM	3165	CZ	ARG	250			119.918	1.00 31.64	В	C
	ATOM	3166	NH1		250			118.839	1.00 32.55	В	И
	MOTA	3167		ARG	250			121.087	1.00 32.97	В	N
	ATOM	3168	C	ARG	250			123.932	1.00 25.34	В	C
45	ATOM	3169	o	ARG	250			124.285	1.00 24.47	В	Ö
70	MOTA	3170	N	LYS	251			124.667	1.00 26.27	В	N
	ATOM	3171	CA	LYS	251			125.963	1.00 27.02	В	C
		3172	CB	LYS	251			126.536	1.00 27.02	В	C
	MOTA	3172	CG	LYS	251			125.798	1.00 27.20	В	C
50	MOTA				251			125.798 L 126.269	1.00 30.10	В	
30	ATOM	3174 3175	CD CE	LYS LYS	251 251			126.269 3 125.419	1.00 32.49	В	C
	ATOM				251 251			9 125.419	1.00 34.43	В	
	ATOM	3176		LYS							N
	ATOM	3177		LYS	251 251			3 126.982 3 127.980		B B	C 0
55	MOTA	3178 3179		LYS	251 252			7 126.739		В	N
55	ATOM			LEU							
	MOTA	3180		LEU	252			2 127.648		В	C
	MOTA	3181		LEU	252			2 127.395			C
	MOTA	3182	CG	LEU	252	9.028	-/2.88	1 127.809	1.00 23.94	B	C

PCT/US2004/023092

	MOTA	3183	CD1		252			127.448	1.00 21.51	В	С
	ATOM	3184	CD2		252			129.317	1.00 22.42	В	C
	MOTA	3185		LEU	252			127.552	1.00 26.17	В	C
_	MOTA	3186	0	LEU	252			128.399	1.00 25.06	В	0
5	ATOM	3187	N	GLN	253			126.525	1.00 26.13	В	N
	MOTA	3188	CA	GLN	253	14.989	-73.571	126.328	1.00 27.67	В	С
	MOTA	3189	CB	GLN	253			127.406	1.00 29.23	В	C
	ATOM	3190	CG	GLN	253	16.176	-71.621	127.559	1.00 32.02	В	С
	MOTA	3191	CD	GLN	253	17.160	-71.282	128.673	1.00 34.60	В	С
10	MOTA	3192	OE1	GLN	253	18.361	-71.531	128.552	1.00 35.64	В	0
	MOTA	3193	NE2	GLN	253	16.651	-70.725	129.770	1.00 35.92	В	N
	MOTA	3194	C	GLN	253	14.859	-75.091	126.392	1.00 27.27	В	C
	MOTA	3195	0	GLN	253	15.553	-75.740	127.170	1.00 27.62	В	0
	MOTA	3196	N	LEU	254	13.979	-75.659	125.578	1.00 26.25	В	N
15	MOTA	3197	CA	LEU	254	13.781	-77.100	125.583	1.00 25.87	В	С
	ATOM	3198	СВ	LEU	254			124.763	1.00 23.25	В	С
	MOTA	3199	CG	LEU	254			125.211	1.00 21.49	В	Ċ
	ATOM	3200		LEU	254			124.364	1.00 20.44	В	C
	MOTA	3201		LEU	254			126.672	1.00 20.62	В	C
20	ATOM	3202	C	LEU	254			125.029	1.00 26.84	В	Č
	MOTA	3203	ō	LEU	254			124.187	1.00 26.79	В	ō
	ATOM	3204	N	GLN	255			125.514	1.00 27.67	В	N
	ATOM	3205	CA	GLN	255			125.037	1.00 29.47	В	c
	ATOM	3206	СВ	GLN	255			126.203	1.00 31.78	В	č
25	ATOM	3207	CG	GLN	255			127.263	1.00 36.11	В	C
	ATOM	3208	CD	GLN	255			128.518	1.00 38.94	В	Č
	ATOM	3209	_	GLN	255			129.476	1.00 40.55	В	Ö
	ATOM	3210	NE2		255			128.523	1.00 39.29	В	N
	ATOM	3211	C	GLN	255			123.952	1.00 33.23	В	C
30	ATOM	3212	Ö	GLN	255			123.954	1.00 28.37	В	Ö
50	ATOM	3212	N	GLU	256			123.934	1.00 28.82	В	N
		3213	CA	GLU	256			123.013	1.00 28.82	В	C
	MOTA MOTA	3214	CB	GLU	256			121.322	1.00 29.58	В	C
	ATOM	3215	CG	GLU	256 256			121.102	1.00 30.58	В	C
35		3217	CD	GLU	256 256			2 119.163	1.00 32.90	В	C
33	ATOM							119.103	1.00 34.07	В	0
	ATOM	3218	OE1 OE2		256 256			117.995	1.00 35.05		
	ATOM	3219			256					В	0
	MOTA	3220	C	GLU	256			1 122.274	1.00 29.06	В	C O
40	MOTA	3221	0	GLU	256			121.677	1.00 29.72 1.00 28.49	В	
40	ATOM	3222	N	PRO	257			123.232	1.00 28.49	В	N C
	ATOM	3223	CD	PRO	257	16.157		5 124.019		В	
	ATOM	3224	CA	PRO	257			2 123.552	1.00 27.78	В	C
	ATOM	3225	CB	PRO	257			124.647	1.00 28.06	В	C
45	ATOM	3226	CG	PRO	257			2 125.201	1.00 29.28	В	C
45	ATOM	3227	C	PRO	257			7 123.958	1.00 26.26	В	C
	MOTA	3228	0	PRO	257			B 123.806	1.00 25.48	В	0
	ATOM	3229	N	GLU	258			0 124.466	1.00 25.25	В	N
	MOTA	3230	CA	GLU	258			2 124.851	1.00 24.25	В	C
F 0	ATOM	3231	CB	GLU	258			7 125.831	1.00 24.97	В	C
50	ATOM	3232	CG	GLU	258			3 127.069		В	C
	ATOM	3233	CD	GLU	258			9 128.029		В	C
	MOTA	3234		L GLU	258			7 127.581		В	0
	MOTA	3235		2 GLU	. 258			4 129.240		В	
EE	ATOM	3236		GLU	258			0 123.587		В	
55	MOTA	3237		GLU				2 123.442			_
	ATOM	3238		TYR				1 122.666			
	ATOM	3239		TYR				4 121.399			
	MOTA	3240	CB	TYR	259	11.939	80.37	8 120.527	1.00 18.72	В	С

-225-

	ATOM	3241	CG	TYR	259		-78.882		1.00 18.66	В	C
	ATOM	3242	CD1	TYR	259	11.074	-77.997	120.378	1.00 18.05	В	C
	MOTA	3243	CE1	TYR	259	11.251	-76.616	120.487	1.00 17.04	В	C
_	MOTA	3244	CD2	TYR	259	13.328	-78.346	121.110	1.00 16.85	В	C
5	ATOM	3245	CE2	TYR	259	13.515	-76.976	121.220	1.00 15.76	В	С
	MOTA	3246	CZ	TYR	259	12.479	-76.114	120.905	1.00 17.18	В	C
	ATOM	3247	OH	TYR	259	12.692	-74.750	120.968	1.00 16.41	В	0
	MOTA	3248	C	TYR	259	10.253	-82.195	120.646	1.00 20.33	В	С
	ATOM	3249	0	TYR	259	9.143	-82.123	120.101	1.00 19.27	В	0
10	ATOM	3250	N	VAL	260	11.009	-83.289	120.618	1.00 20.16	В	N
	MOTA	3251	CA	VAL	260	10.588	-84.498	119.930	1.00 22.13	В	С
	MOTA	3252	CB	VAL	260	11.730	-85.535	119.921	1.00 24.17	В	C
	MOTA	3253	CG1	VAL	260	11.205	-86.882	119.500	1.00 24.73	В	C
	MOTA	3254	CG2	VAL	260	12.822	-85.088	118.949	1.00 25.03	В	С
15	MOTA	3255	С	VAL	260	9.324	-85.119	120.530	1.00 21.91	В	C
	MOTA	3256	0	VAL	260	8.428	-85.541	119.796	1.00 21.90	В	0
	MOTA	3257	N	LEU	261	9.249	-85.181	121.855	1.00 21.23	В	N
	MOTA	3258	CA	LEU	261	8.074	-85.746	122.516	1.00 22.69	В	С
	MOTA	3259	CB	LEU	261	8.334	-85.912	124.019	1.00 22.40	В	С
20	MOTA	3260	CG	LEU	261	9.193	-87.127	124.378	1.00 22.56	В	C
	MOTA	3261	CD1	LEU	261	9.560	-87.121	125.861	1.00 23.42	В	C
	ATOM	3262	CD2	LEU	261	8.419	-88.390	124.019	1.00 21.06	В	C
	MOTA	3263	С	LEU	261	6.842	-84.869	122.283	1.00 22.97	В	С
	MOTA	3264	0	LEU	261	5.721	-85.365	122.182	1.00 23.28	В	0
25	MOTA	3265	N	LEU	262	7.063	-83.565	122.191	1.00 22.71	В	N
	MOTA	3266	CA	LEU	262	5.992	-82.611	121.950	1.00 23.51	В	С
	MOTA	3267	CB	LEU	262	6.568	-81.194	122.027	1.00 24.71	В	С
	ATOM	3268	CG	LEU	262	5.647	-80.042	122.429	1.00 27.53	В	C
	MOTA	3269	CD1	LEU	262	5.105	-80.278	123.839	1.00 27.55	В	С
30	MOTA	3270	CD2	LEU	262	6.427	-78.733	122.369	1.00 27.91	В	C
	MOTA	3271	C	LEU	262	5.396	-82.889	120.555	1.00 23.38	В	С
	ATOM	3272	0	LEU	262	4.170	-82.918	120.376	1.00 22.75	В	0
	MOTA	3273	N	ALA	263	6.270	-83.100	119.572	1.00 22.06	В	N
	MOTA	3274	CA	ALA	263	5.834	-83.399	118.215	1.00 22.18	В	C
35	MOTA	3275	СВ	ALA	263	7.036	-83.499	117.285	1.00 20.60	В	С
	ATOM	3276	C	ALA	263	5.071	-84.722	118.231	1.00 22.24	В	C
	MOTA	3277	0	ALA	263	4.030	-84.852	117.585	1.00 22.01	В	0
	MOTA	3278	N	ALA	264	5.593	-85.702	118.965	1.00 21.91	В	N
	MOTA	3279	CA	ALA	264	4.938	-87.005	119.073	1.00 22.99	В	C
40	MOTA	3280	CB	ALA	264			119.905	1.00 23.25	В	C
	MOTA	3281	C	ALA	264			119.707	1.00 23.31	В	C
	MOTA	3282	0	ALA	264			119.307	1.00 23.47	В	0
	ATOM	3283	N	MET	265			120.702	1.00 23.39	В	N
4.5	ATOM	3284	CA	MET	265			121.359	1.00 24.89	В	C
45	ATOM	3285	CB	MET	265			122.617	1.00 26.27	В	C
	MOTA	3286	CG	MET	265			123.761	1.00 28.18	В	С
	MOTA	3287	SD	MET	265			125.239	1.00 30.04	В	S
	MOTA	3288	CE	MET	265			125.842	1.00 28.25	В	С
50	MOTA	3289	С	MET	265			120.415	1.00 24.62	В	С
50	MOTA	3290	0	MET	265			120.487	1.00 24.02	В	0
	MOTA	3291	N	ALA	266			3 119.531	1.00 24.92	В	N
	MOTA	3292	CA	ALA	266			3 118.550	1.00 25.19	В	С
	MOTA	3293	СВ	ALA	266			117.835	1.00 23.17	В	C
EF	MOTA	3294	С	ALA	266			3 117.532	1.00 25.75	В	С
55	MOTA	3295	0	ALA	266			117.156	1.00 25.62	В	0
	MOTA	3296	N	LEU	267			117.092	1.00 25.83	В	N
	MOTA	3297	CA	LEU	267			1 116.123		В	С
	ATOM	3298	CB	LEU	267	2.296	-87.377	7 115.891	1.00 26.43	В	C

WO 2005/019239 PCT/US2004/023092

-226-

	MOTA	3299		LEU	267	2.542 -88.069 114.541 1.00 27.28 B C
	MOTA	3300	CD1	_	267	3.607 -89.134 114.721 1.00 26.00 B C
	MOTA	3301	CD2		267	1.281 -88.692 113.999 1.00 27.86 B C
_	MOTA	3302		LEU	267	-0.081 -87.505 116.596 1.00 27.40 B C
5	MOTA	3303		LEU	267	-1.059 -87.741 115.883 1.00 27.12 B O
	MOTA	3304		PHE	268	0.084 -88.047 117.799 1.00 28.25 B N
	MOTA	3305	CA	PHE	268	-0.876 -89.006 118.341 1.00 30.10 B C
	MOTA	3306	CB	PHE	268	-0.145 -90.017 119.233 1.00 28.85 B C
	MOTA	3307	CG	PHE	268	0.824 -90.889 118.483 1.00 28.85 B C
10	ATOM	3308	CD1		268	2.184 -90.857 118.777 1.00 28.83 B C
	ATOM	3309	CD2		268	0.380 -91.709 117.451 1.00 28.35 B C
	MOTA	3310		PHE	268	3.091 -91.629 118.047 1.00 30.17 B C
	MOTA	3311		PHE	268	1.276 -92.486 116.713 1.00 29.06 B C
	MOTA	3312	CZ	PHE	268	2.635 -92.447 117.008 1.00 28.98 B C
15	MOTA	3313	С	PHE	268	-2.078 -88.427 119.084 1.00 31.65 B C
	MOTA	3314	0	PHE	268	-2.299 -88.727 120.255 1.00 31.36 B O
	MOTA	3315	N	SER	269	-2.858 -87.611 118.386 1.00 34.17 B N
	MOTA	3316	CA	SER	269	-4.054 -87.004 118.961 1.00 36.81 B C
	MOTA	3317	CB	SER	269	-4.240 -85.581 118.435 1.00 36.42 B C
20	MOTA	3318	OG	SER	269	-3.138 -84.767 118.789 1.00 37.62 B O
	MOTA	3319	C	SER	269	-5.260 -87.854 118.566 1.00 38.85 B C
	MOTA	3320	0	SER	269	-5.567 -87.996 117.380 1.00 38.42 B O
	MOTA	3321	N	PRO	270	-5.959 -88.428 119.561 1.00 40.51 B N
	MOTA	3322	CD	PRO	270	-5.665 -88.310 121.002 1.00 40.82 B C
25	ATOM	3323	CA	PRO	270	-7.138 -89.275 119.336 1.00 41.97 B C
	MOTA	3324	CB	PRO	270	-7.342 -89.938 120.695 1.00 41.86 B C
	MOTA	3325	CG	PRO	270	-6.941 -88.839 121.643 1.00 41.56 B C
	MOTA	3326	С	PRO	270	-8.391 -88.532 118.871 1.00 43.29 B C
	ATOM	3327	0	PRO	270	-9.311 -89.141 118.325 1.00 43.76 B O
30	MOTA	3328	N	ASP	271	-8.429 -87.222 119.088 1.00 44.33 B N
	ATOM	3329	CA	ASP	271	-9.585 -86.424 118.696 1.00 45.68 B C
	ATOM	3330	CB	ASP	271	-9.881 -85.370 119.774 1.00 46.97 B C
	MOTA	3331	CG	ASP	271	-8.764 -84.350 119.928 1.00 48.52 B C
	MOTA	3332	OD1	ASP	271	-7.578 -84.724 119.795 1.00 49.44 B O
35	MOTA	3333	OD2	ASP	271	-9.075 -83.168 120.202 1.00 49.05 B O
	MOTA	3334	C	ASP	271	-9.389 -85.765 117.334 1.00 45.97 B C
	MOTA	3335	0	ASP	271	-9.848 -84.651 117.089 1.00 45.91 B O
	ATOM	3336	N	ARG	272	-8.707 -86.476 116.444 1.00 45.79 B N
	MOTA	3337	CA	ARG	272	-8.448 -85.977 115.108 1.00 45.77 B C
40	MOTA	3338	CB	ARG	272	-7.094 -86.489 114.612 1.00 44.26 B C
	MOTA	3339	CG	ARG	272	-6.217 -85.425 113.998 1.00 41.89 B C
	MOTA	3340	CD	ARG	272	-5.168 -84.917 114.976 1.00 39.65 B C
	MOTA	3341	NE	ARG	272	-5.198 -83.463 115.076 1.00 38.37 B N
45	MOTA	3342	CZ	ARG	272	-4.192 -82.703 115.503 1.00 37.88 B C
45	MOTA	3343		ARG	272	-3.037 -83.239 115.876 1.00 37.41 B N
	MOTA	3344		ARG	272	-4.351 -81.392 115.565 1.00 36.36 B N
	MOTA	3345	С	ARG	272	-9.552 -86.476 114.182 1.00 46.79 B C
	MOTA	3346	0	ARG	272	-9.843 -87.671 114.135 1.00 46.53 B O
	MOTA	3347	N	PRO	273	-10.185 -85.564 113.432 1.00 47.81 B N
50	ATOM	3348		PRO	273	-9.883 -84.133 113.255 1.00 48.15 B C
	MOTA	3349		PRO	273	-11.252 -85.992 112.525 1.00 48.97 B C
	MOTA	3350		PRO	273	-11.603 -84.704 111.772 1.00 48.79 B C
	MOTA	3351		PRO	273	-10.332 -83.897 111.838 1.00 48.65 B C
	MOTA	3352		PRO	273	-10.813 -87.125 111.594 1.00 49.83 B C
55	MOTA	3353		PRO	273	-9.809 -87.009 110.890 1.00 49.98 B O
	MOTA	3354		GLY	274	-11.566 -88.223 111.615 1.00 50.41 B N
	MOTA	3355		GLY	274	-11.257 -89.363 110.769 1.00 51.30 B C
	MOTA	3356	C	GLY	274	-10.578 -90.544 111.443 1.00 52.28 B C

-227-

	ATOM	3357		GLY	274	-10.367			1.00 52.21	В	0
	MOTA	3358		VAL	275	-10.234			1.00 53.24	В	N
	MOTA	3359		VAL	275		-91.500		1.00 54.29	В	C
_	MOTA	3360		VAL	275		-90.984		1.00 54.20	В	C
5	MOTA	3361	CG1		275		-90.054		1.00 54.52	В	C
	MOTA	3362		VAL	275		-90.268		1.00 54.74	В	C
	MOTA	3363		VAL	275	-10.525			1.00 54.76	В	C
	MOTA	3364		VAL	275		-92.348		1.00 54.98	В	0
40	MOTA	3365		THR	276		-93.835		1.00 55.29	В	N
10	MOTA	3366		THR	276		-95.014		1.00 55.88	В	С
	MOTA	3367		THR	276		-96.152		1.00 55.89	В	C
	MOTA	3368	OG1		276		-95.665		1.00 55.88	В	0
	ATOM	3369		THR	276		-97.315		1.00 56.57	В	C
45	ATOM	3370	C	THR	276		-95.527		1.00 56.10	В	C
15	ATOM	3371		THR	276		-95.625	116.173	1.00 56.37	В	0
	MOTA	3372	N	GLN	277			115.387	1.00 56.20	В	N
	ATOM	3373	CA	GLN	277			116.618	1.00 56.61	В	C
	MOTA	3374	СВ	GLN	277			116.292	1.00 57.07	В	C
00	MOTA	3375	CG	GLN	277			116.026	1.00 58.02	В	C
20	MOTA	3376	CD	GLN	277			115.228	1.00 58.03	В	C
	MOTA	3377	OE1		277			114.126	1.00 59.02	В	0
	MOTA	3378	NE2		277			115.784	1.00 58.06	В	N
	MOTA	3379	C	GLN	277			117.707	1.00 56.48	В	С
05	MOTA	3380	0	GLN	277			118.130	1.00 56.27	В	0
25	ATOM	3381	N	ARG	278			118.172	1.00 56.44	В	N
	ATOM	3382	CA	ARG	278			119.205	1.00 56.32	В	C
	MOTA	3383	CB	ARG	278			119.574	1.00 57.69	В	С
	MOTA	3384	CG	ARG	278			118.495	1.00 59.91	В	C
20	MOTA	3385	CD	ARG	278			119.105	1.00 62.28	В	С
30	ATOM	3386	NE	ARG	278			119.921	1.00 64.42	В	N
	ATOM	3387	CZ	ARG	278			120.534	1.00 65.26	В	С
	MOTA	3388	NH1		278			120.436	1.00 65.68	В	N
	MOTA	3389	NH2		278			121.243	1.00 65.69	В	N
25	MOTA	3390	С	ARG	278			120.467	1.00 55.50	В	С
35	ATOM	3391	0	ARG	278			120.850	1.00 55.10	В	0
	MOTA	3392	N	ASP	279			121.116	1.00 54.66	В	Ŋ
	MOTA	3393	CA	ASP	279			122.337	1.00 54.08	В	C
	ATOM	3394	CB	ASP	279			122.869	1.00 55.13	В	C
40	ATOM	3395	CG	ASP	279			123.205	1.00 56.06	В	C
40	ATOM	3396		ASP	279			123.898	1.00 56.83	B B	0
	ATOM	3397 3398		ASP ASP	279			122.782	1.00 56.30 1.00 53.02	В	C
	ATOM		C		279			122.102			_
	ATOM	3399	0	ASP	279 280			122.928	1.00 52.50 1.00 52.25	В	0
45	MOTA	3400		GLU				120.571	1.00 52.25	В	N
70	ATOM	3401	CA	GLU	280					В	C
	ATOM	3402		GLU	280			9 119.221 5 119.136	1.00 53.05 1.00 55.94	B B	C
	ATOM	3403		GLU	280			119.130	1.00 57.54		C
	MOTA	3404		GLU	280 280			118.794	1.00 57.75		0
50	MOTA	3405			280			3 120.271	1.00 57.75		
30	MOTA	3406									
	ATOM	3407		GLU	280			1 120.605 5 121.211	1.00 49.94		
	MOTA	3408		GLU	280				1.00 49.12		
	MOTA	3409		ILE	281			2 119.919 2 119.827	1.00 48.25		
55	MOTA	3410		ILE	281						
<i>3</i> 3	MOTA	3411		ILE	281			2 118.660 4 118 645			
	MOTA	3412		ILE	281			4 118.645 5 117 33 <i>4</i>			
	MOTA	3413		. ILE	281			6 117.334 2 116 116			
	MOTA	3414	CD1	ILE	281	-4.913	-92.80.	3 116.116	1.00 45.69	B	С

-228-

	MOTA	3415	C	ILE	281		-92.912		1.00 46.37	В	C
	MOTA	3416	0	ILE	281		-92.248		1.00 46.02	В	0
	MOTA	3417	N	ASP	282		-92.986		1.00 46.17	В	N
_	ATOM	3418	CA	ASP	282		-92.272		1.00 45.94	В	C
5	MOTA	3419	CB	ASP	282		-92.451		1.00 46.56	В	С
	MOTA	3420	CG	ASP	282		-91.618		1.00 48.23	В	C
	MOTA	3421	OD1		282		-90.381		1.00 48.42	В	0
	MOTA	3422	OD2		282		-92.197		1.00 48.95	В	0
40	MOTA	3423	С	ASP	282		-92.780		1.00 45.01	В	С
10	MOTA	3424	0	ASP	282		-92.000		1.00 45.05	В	0
	MOTA	3425	N	GLN	283		-94.088		1.00 44.59	В	N
	MOTA	3426	CA	GLN	283			124.994	1.00 43.67	В	C
	MOTA	3427	CB	GLN	283			124.999	1.00 45.52	В	C
	ATOM	3428	CG	GLN	283			125.705	1.00 48.81	В	C
15	MOTA	3429	CD	GLN	283	-4.612	-98.206	125.633	1.00 51.03	В	C
	MOTA	3430	OE1	GLN	283	-3.712	-98.967	126.000	1.00 52.12	В	0
	MOTA	3431	NE2	GLN	283	-5.778	-98.646	125.162	1.00 51.60	В	N
	MOTA	3432	C	GLN	283	-1.601	-94.328	124.550	1.00 41.87	В	C
	MOTA	3433	0	GLN	283	-0.710	-94.154	125.376	1.00 40.63	В	0
20	MOTA	3434	N	LEU	284	-1.395	-94.218	123.243	1.00 40.30	В	N
	ATOM	3435	CA	LEU	284	-0.085	-93.856	122.718	1.00 39.29	В	C
	ATOM	3436	CB	LEU	284			121.185	1.00 39.37	В	C
	MOTA	3437	CG	LEU	284			120.550	1.00 39.93	В	C
	MOTA	3438	CD1	LEU	284	-0.345	-96.415	121.249	1.00 40.63	В	C
25	MOTA	3439	CD2	LEU	284	-0.001	-95.239	119.067	1.00 38.88	В	С
	MOTA	3440	С	LEU	284	0.303	-92.456	123.188	1.00 37.95	В	C
	MOTA	3441	0	LEU	284	1.425	-92.231	123.638	1.00 37.80	В	0
	MOTA	3442	N	GLN	285	-0.625	-91.514	123.092	1.00 36.96	В	N
	MOTA	3443	CA	GLN	285	-0.326	-90.164	123.529	1.00 36.82	В	C
30	MOTA	3444	CB	GLN	285			123.239	1.00 37.92	В	C
	MOTA	3445	CG	GLN	285	-1.222	-87.811	123.761	1.00 39.28	В	C
	ATOM	3446	CD	GLN	285			123.334	1.00 40.09	В	C
	MOTA	3447	OE1		285	-2.244	-86.323	122.218	1.00 41.73	В	0
	ATOM	3448	NE2	GLN	285	-3.241	-86.594	124.211	1.00 40.92	В	N
35	MOTA	3449	С	GLN	285			125.016	1.00 36.21	В	C
	MOTA	3450	0	GLN	285			125.436	1.00 34.84	В	0
	MOTA	3451	N	GLU	286			125.810	1.00 35.91	В	N
	MOTA	3452	CA	GLU	286			127.249	1.00 36.06	В	C
4.0	MOTA	3453	CB	GLU	286			127.937	1.00 38.35	В	C
40	MOTA	3454	CG	GLU	286			129.446	1.00 42.49	В	С
	MOTA	3455	CD	GLU	286	-1.209	-90.639	130.124	1.00 44.67	В	C
	MOTA	3456	OE1	. GLU	286			129.837	1.00 46.65	В	0
	MOTA	3457		GLU	286			. 130.950	1.00 46.57	В	0
	MOTA	3458	C	GLU	286			127.499	1.00 35.04	В	С
45	MOTA	3459	0	GLU	286			128.387	1.00 34.20	В	0
	ATOM	3460	N	GLU	287			126.708	1.00 34.29	В	N
	MOTA	3461	CA	GLU	287			126.823	1.00 33.78	В	C
	ATOM	3462	CB	GLU	287			125.851	1.00 35.48	В	C
	MOTA	3463	CG	GLU	287			125.864	1.00 38.18	В	С
50	MOTA	3464	CD	GLU	287			2 124.964	1.00 40.29	В	C
	MOTA	3465		GLU	287			124.870		В	0
	MOTA	3466		GLU	287			l 124.354		В	0
	MOTA	3467	С	GLU	287			126.506		В	
	MOTA	3468	0	GLU	287			l 127.157		В	
55	MOTA	3469	N	MET	288			3 125.499		В	N
	MOTA	3470		MET	288			3 125.129		В	С
	MOTA	3471		MET	288			9 123.883		В	_
	MOTA	3472	CG	MET	288	3.437	-90.03	l 122.645	1.00 30.98	В	С

-229-

	ATOM	3473	SD	MET	288	4.901	-90.867	122.003	1.00 33.03	В	S
	MOTA	3474	CE	MET	288	4.384	-92.607	122.202	1.00 32.43	В	С
	MOTA	3475	С	MET	288	4.251	-88.919	126.300	1.00 28.89	В	C
	MOTA	3476	0	MET	288	5.310	-88.489	126.751	1.00 28.59	В	0
5	ATOM	3477	N	ALA	289	3.065	-88.568	126.786	1.00 28.24	В	N
	MOTA	3478	CA	ALA	289	2.920	-87.622	127.887	1.00 28.40	В	С
	ATOM	3479	CB	ALA	289	1.441	-87.415	128.195	1.00 27.31	В	C
	ATOM	3480	C	ALA	289	3.674	-88.059	129.146	1.00 28.77	В	С
	ATOM	3481	0	ALA	289	4.356	-87.248	129.777	1.00 28.99	В	0
10	MOTA	3482	N	LEU	290	3.555	-89.333	129.511	1.00 29.19	В	N
	ATOM	3483	CA	LEU	290	4.248	-89.850	130.688	1.00 29.74	В	C
	MOTA	3484	CB	LEU	290	3.786	-91.271	131.019	1.00 31.00	В	С
	ATOM	3485	CG	LEU	290	2.366	-91.417	131.574	1.00 33.11	В	С
	ATOM	3486	CD1	LEU	290	2.029	-92.895	131.750	1.00 33.94	В	С
15	MOTA	3487		LEU	290			132.908	1.00 34.21	В	С
	MOTA	3488	С	LEU	290	5.750	-89.850	130.475	1.00 29.25	В	C
	ATOM	3489	0	LEU	290	6.510	-89.582	131.400	1.00 29.29	В	0
	ATOM	3490	N	THR	291	6.183	-90.158	129.255	1.00 28.88	В	N
	ATOM	3491	CA	THR	291			128.959	1.00 27.56	В	С
20	ATOM	3492	CB	THR	291	7.886	-90.695	127.538	1.00 27.69	В	C
	ATOM	3493	OG1		291	7.381	-92.034	127.419	1.00 27.19	В	0
	ATOM	3494	CG2		291			127.248	1.00 25.40	В	C
	ATOM	3495	C	THR	291			129.090	1.00 27.38	В	Č
	ATOM	3496	ŏ	THR	291			129.637	1.00 26.70	В	ō
25	ATOM	3497	N	LEU	292			128.586	1.00 26.91	В	N
	ATOM	3498	CA	LEU	292			128.681	1.00 27.05	В	C
	ATOM	3499	СВ	LEU	292			127.928	1.00 25.96	В	Č
	ATOM	3500	CG	LEU	292			127.939	1.00 25.61	В	Ċ
	ATOM	3501	-	LEU	292			127.580	1.00 23.77	В	Č
30	ATOM	3502		LEU	292			126.966	1.00 24.54	В	C
•	ATOM	3502	C	LEU	292			130.151	1.00 27.73	В	c
	ATOM	3504	ŏ	LEU	292			130.554	1.00 26.74	В	ŏ
	ATOM	3505	N	GLN	293			130.949	1.00 29.30	В	N
	ATOM	3506	CA	GLN	293			132.374	1.00 31.80	В	C
35	ATOM	3507	СВ	GLN	293			133.059	1.00 33.01	В	C
•	ATOM	3508	CG	GLN	293			132.675	1.00 35.44	В	Č
	MOTA	3509	CD	GLN	293	3.151		133.354	1.00 37.29	В	C
	ATOM	3510	OE1		293	3.067		134.588	1.00 36.31	В	ŏ
	MOTA	3511	NE2		293	2.201		132.546	1.00 38.33	В	N
40	ATOM	3512	C	GLN	293			133.051	1.00 32.77	В	C
	ATOM	3513	ŏ	GLN	293			133.707	1.00 32.11	В	ō
	ATOM	3514	N	SER	294			132.881	1.00 33.57	В	N
	ATOM	3515	CA	SER	294			2 133.460	1.00 34.88	В	C
	MOTA	3516	СВ	SER	294			3 132.962	1.00 34.00	В	Ċ
45	MOTA	3517	OG	SER	294			3 133.261	1.00 37.51	В	Ö
.0	ATOM	3518	c	SER	294			3 133.090	1.00 34.78	В	č
	ATOM	3519	Ö	SER	294			l 133.947	1.00 34.65	В	o
	ATOM	3520	N	TYR	295			3 131.805	1.00 34.99	В	N
	ATOM	3521	CA	TYR	295			131.331	1.00 35.00	В	C
50	ATOM	3522	CB	TYR	295			9 129.814	1.00 34.20	В	C
50	MOTA	3523	CG	TYR				5 129.263	1.00 33.37	В	c
	ATOM	3523		l TYR				6 129.289	1.00 33.57	В	C
		3524 3525		L TYR				6 129.289 6 128.811	1.00 32.31	В	C
	MOTA MOTA	3525 3526		2 TYR				8 128.741		В	C
55	ATOM	3526 3527		2 TYR				9 128.260		В	C
-	ATOM	3528	CZ.	TYR				9 128.295		В	
	ATOM	3529						5 128.295 5 127.784			
										В	
	ATOM	3530	C	TYR	295	12.39	L -00.09	8 131.993	1.00 33.91	D	C

-230-

	ATOM	3531	0	TYR	295	13.510	-85.268	132.379	1.00 35.15	В	0
	MOTA	3532	N	ILE	296	11.327	-84.809	132.111	1.00 37.71	В	N
	MOTA	3533	CA	ILE	296	11.418	-83.492	132.741	1.00 40.23	В	C
	ATOM	3534	CB	ILE	296	10.084	-82.705	132.618	1.00 39.25	В	C
5	MOTA	3535		ILE	296	10.153	-81.424	133.447	1.00 38.18	В	C
	MOTA	3536	CG1	ILE	296	9.797	-82.378	131.151	1.00 38.83	В	C
	MOTA	3537	CD1	ILE	296	8.486	-81.651	130.932	1.00 38.48	В	С
	MOTA	3538	C	ILE	296	11.751	-83.639	134.227	1.00 42.98	В	C
	ATOM	3539	0	ILE	296	12.617	-82.934	134.752	1.00 42.72	В	0
10	MOTA	3540	N	LYS	297	11.050	-84.552	134.897	1.00 46.09	В	N
	ATOM	3541	CA	LYS	297	11.263	-84.799	136.317	1.00 49.98	В	C
	ATOM	3542	CB	LYS	297	10.432	-85.997	136.786	1.00 49.95	В	C
	ATOM	3543	CG	LYS	297	8.949	-85.718	136.966	1.00 50.90	В	C
	ATOM	3544	CD	LYS	297	8.231	-86.957	137.487	1.00 51.71	В	С
15	MOTA	3545	CE	LYS	297	6.745	-86.713	137.702	1.00 51.90	В	C
	MOTA	3546	NZ	LYS	297			138.193	1.00 52.46	В	N
	ATOM	3547	С	LYS	297			136.632	1.00 52.54	В	C
	ATOM	3548	0	LYS	297	13.306	-84.405	137.500	1.00 53.13	В	0
	ATOM	3549	N	GLY	298	13.335	-85.998	135.919	1.00 55.39	В	N
20	ATOM	3550	CA	GLY	298			136.167	1.00 59.24	В	C
	ATOM	3551	C	GLY	298			135.485	1.00 62.03	В	C
	ATOM	3552	0	GLY	298			135.824	1.00 62.62	В	ō
	ATOM	3553	N	GLN	299			134.536	1.00 64.81	В	N
	ATOM	3554	CA	GLN	299			133.816	1.00 67.60	В	C
25	ATOM	3555	CB	GLN	299			132.688	1.00 67.76	В	c
_	ATOM	3556	CG	GLN	299			131.729	1.00 68.45	В	Ċ
	ATOM	3557	CD	GLN	299			131.453	1.00 68.63	В	c
	MOTA	3558	OE1		299			131.236	1.00 68.95	В	ō
	ATOM	3559	NE2		299			131.457	1.00 68.63	В	N
30	ATOM	3560	С	GLN	299			134.697	1.00 69.34	В	C
	ATOM	3561	ō	GLN	299			135.518	1.00 69.59	В	o
	ATOM	3562	N	GLN	300			134.495	1.00 71.45	В	N
	ATOM	3563	CA	GLN	300			135.221	1.00 73.26	В	C
	ATOM	3564	СВ	GLN	300			134.676	1.00 73.69	В	č
35	ATOM	3565	CG	GLN	300			135.213	1.00 74.64	В	C
	ATOM	3566	CD	GLN	300			134.846	1.00 75.14	В	C
	ATOM	3567		GLN	300			133.667	1.00 75.32	В	ŏ
	ATOM	3568		GLN	300			135.858	1.00 75.53	В	N
	ATOM	3569	C	GLN	300			135.204	1.00 74.21	В	Ċ
40	ATOM	3570	ō	GLN	300			135.303	1.00 74.60	В	ŏ
. •	ATOM	3571	N	ARG	301			135.073	1.00 75.01	В	N
	ATOM	3572	CA	ARG	301			135.086		В	
	ATOM	3573	CB	ARG	301			133.858	1.00 75.26	В	C
	ATOM	3574	CG	ARG	301			133.901	1.00 75.18	В	c
45	ATOM	3575	CD	ARG	301			132.580	1.00 75.06	В	c
. •	ATOM	3576	NE	ARG	301			132.349	1.00 74.97	В	N
	ATOM	3577	CZ	ARG	301			31.281	1.00 74.61	В	C
	ATOM	3578		ARG	301			130.317	1.00 74.17	В	N
	ATOM	3579		ARG	301			3 131.174	1.00 74.08	В	N
50	MOTA	3580	C	ARG	301			136.384	1.00 75.55	В	C
•	ATOM	3581	ō	ARG	301			136.615	1.00 75.54	В	ō
	ATOM	3582	Ŋ	ARG	302			5 137.240	1.00 75.70	В	N
	ATOM	3583	CA	ARG	302			138.507	1.00 75.70	В	C
	ATOM	3584	СВ	ARG	302			3 139.602	1.00 76.38	В	C
55	ATOM	3585	CG	ARG	302			5 141.018		В	C
_ •	ATOM	3586		ARG				7 141.988		В	C
	ATOM	3587		ARG	302			7 142.207		В	N
	ATOM	3588		ARG	302			142.207		В	C
	OF1	2200	C2	פאה	J U Z	21.002	-13.23	745.000	1.00 /0.20	D	C

-231-

	ATOM	3589	NH1		302	20.507 -74.674 143.391 1.00 78.27 B	N
	MOTA	3590		ARG	302	22.767 -74.760 143.016 1.00 78.37 B	N
	MOTA	3591		ARG	302	17.762 -75.317 138.574 1.00 75.23 B	C
_	MOTA	3592		ARG	302	17.499 -74.803 139.663 1.00 75.35 B	0
5	MOTA	3593		PRO	303	17.202 -74.860 137.430 1.00 74.61 B	N
	MOTA	3594	CD	PRO	303	17.298 -75.150 135.986 1.00 74.54 B	С
	MOTA	3595	CA	PRO	303	16.273 -73.750 137.667 1.00 73.58 B	C
	MOTA	3596	СВ	PRO	303	16.012 -73.215 136.261 1.00 73.72 B	С
	MOTA	3597	CG	PRO	303	16.073 -74.451 135.427 1.00 74.08 B	C
10	ATOM	3598	С	PRO	303	15.010 -74.319 138.321 1.00 72.47 B	С
	MOTA	3599	0	PRO	303	14.156 -73.579 138.807 1.00 72.47 B	0
	MOTA	3600	N	ARG	304	14.920 -75.648 138.330 1.00 71.25 B	N
	MOTA	3601	CA	ARG	304	13.796 -76.366 138.901 1.00 69.81 B	C
	MOTA	3602	CB	ARG	304	13.947 -76.484 140.423 1.00 71.29 B	С
15	MOTA	3603		ARG	304	14.821 -77.652 140.877 1.00 72.92 B	С
	ATOM	3604		ARG	304	14.673 -77.891 142.376 1.00 74.32 B	С
	ATOM	3605	NE	ARG	304	15.207 -79.188 142.794 1.00 75.67 B	N
	MOTA	3606	CZ	ARG	304	15.103 -79.684 144.027 1.00 76.25 B	С
	ATOM	3607	NH1	ARG	304	14.484 -78.995 144.980 1.00 76.56 B	N
20	MOTA	3608	NH2		304	15.613 -80.876 144.309 1.00 76.34 B	
	MOTA	3609	С	ARG	304	12.464 -75.716 138.562 1.00 67.71 B	
	MOTA	3610	0	ARG	304	11.882 -74.999 139.379 1.00 68.11 B	
	MOTA	3611	N	ASP	305	11.989 -75.956 137.344 1.00 64.75 B	
	MOTA	3612	CA	ASP	305	10.708 -75.417 136.929 1.00 61.23 B	
25	MOTA	3613	СВ	ASP	305	10.789 -74.800 135.534 1.00 61.94 B	
	MOTA	3614	CG	ASP	305	9.459 -74.232 135.082 1.00 62.41 B	
	MOTA	3615	OD1	ASP	305	8.677 -73.803 135.959 1.00 62.77 B	
	ATOM	3616	OD2	ASP	305	9.202 -74.194 133.860 1.00 62.51 B	0
	ATOM	3617	С	ASP	305	9.679 -76.536 136.956 1.00 58.50 B	
30	ATOM	3618	0	ASP	305	9.625 -77.382 136.059 1.00 58.07 B	
	ATOM	3619	N	ARG	306	8.878 -76.543 138.016 1.00 54.93 B	
	MOTA	3620	CA	ARG	306	7.840 -77.548 138.187 1.00 51.10 B	C
	MOTA	3621	CB	ARG	306	7.408 -77.604 139.651 1.00 53.42 B	C
4	MOTA	3622	CG	ARG	306	8.513 -77.985 140.611 1.00 56.34 B	C
35	MOTA	3623	CD	ARG	306	8.016 -77.954 142.041 1.00 59.35 B	C
	ATOM	3624	NE	ARG	306	9.051 -78.364 142.988 1.00 61.82 B	N
	MOTA	3625	CZ	ARG	306	8.925 -78.298 144.308 1.00 62.64 E	C
	MOTA	3626	NH1	ARG	306	9.923 -78.686 145.090 1.00 62.90 E	N
	ATOM	3627	NH2	ARG	306	7.805 -77.831 144.840 1.00 63.33 E	
40	ATOM	3628	С	ARG	306	6.644 -77.204 137.318 1.00 46.82 E	C
	ATOM	3629	0	ARG	306	5.683 -77.962 137.241 1.00 46.07 E	3 0
	ATOM	3630	N	PHE	307		3 N
	MOTA	3631	CA	PHE	307	5.647 -75.583 135.807 1.00 38.22 E	
	MOTA	3632	CB	PHE	307	5.481 -74.068 135.962 1.00 38.24 E	
45	MOTA	3633	CG	PHE	307	5.179 -73.628 137.369 1.00 38.97 E	
	MOTA	3634		PHE	307	6.188 -73.556 138.326 1.00 39.66 E	
	MOTA	3635		PHE	307	3.883 -73.296 137.741 1.00 39.64 E	
	ATOM	3636		PHE	307	5.915 -73.160 139.632 1.00 40.08 E	
=0	MOTA	3637	CE2		307	3.595 -72.898 139.047 1.00 40.42 E	
50	MOTA	3638	CZ	PHE	307		3 C
	MOTA	3639		PHE	307		3 C
	ATOM	3640	0	PHE	307		3 0
	MOTA	3641	N	LEU	308		3 17
EF	ATOM	3642		LEU	308		3 C
55	ATOM	3643		LEU	308		3 C
	ATOM	3644		LEU	308		3 C
	ATOM	3645		LEU	308		3 C
	MOTA	3646	CD2	LEU	308	8.932 -77.041 130.142 1.00 30.29	3 C

-232-

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	MOTA	3647	C	LEU	308	6.420 -77.671 131.956 1.00 27.96 B C	
	MOTA	3648	0	LEU	308	5.892 -77.296 130.911 1.00 26.38 B O	
	MOTA	3649	N	TYR	309	6.146 -78.847 132.517 1.00 26.33 B N	
_	MOTA	3650	CA	TYR	309	5.199 -79.770 131.896 1.00 26.08 B C	
5	MOTA	3651	CB	TYR	309	5.037 -81.040 132.743 1.00 26.27 B C	
	MOTA	3652	CG	TYR	309	4.121 -82.074 132.109 1.00 26.57 B C	;
	MOTA	3653	CD1	TYR	309	4.409 -82.611 130.855 1.00 26.55 B C	,
	ATOM	3654	CE1	TYR	309	3.559 -83.533 130.249 1.00 27.76 B C	:
	ATOM	3655	CD2	TYR	309	2.955 -82.489 132.749 1.00 26.42 B C	
10	MOTA	3656	CE2	TYR	309	2.092 -83.414 132.152 1.00 28.03 B C	
	ATOM	3657	CZ	TYR	309	2.404 -83.930 130.902 1.00 27.91 B C	
	ATOM	3658	ОН	TYR	309	1.568 -84.847 130.312 1.00 29.13 B C	
	ATOM	3659	C	TYR	309	3.830 -79.135 131.650 1.00 25.30 B	
	ATOM	3660	ŏ	TYR	309	3.261 -79.280 130.568 1.00 24.69 B	
15	ATOM	3661	N	ALA	310	3.308 -78.427 132.649 1.00 24.77 B	
	ATOM	3662	CA	ALA	310		
	MOTA	3663	CB	ALA	310	2.007 -77.780 132.519 1.00 23.64 B C 1.628 -77.092 133.822 1.00 24.37 B C	
			-				
	ATOM	3664	C	ALA	310	2.047 -76.764 131.385 1.00 23.22 B	
20	MOTA	3665	0	ALA	310	1.088 -76.630 130.628 1.00 22.01 B	
20	MOTA	3666	N	LYS	311	3.158 -76.043 131.276 1.00 22.47 B N	
	MOTA	3667	CA	LYS	311	3.315 -75.052 130.217 1.00 22.76 B	
	ATOM	3668	CB	LYS	311	4.612 -74.271 130.413 1.00 23.73 B	
	MOTA	3669	CG	LYS	311	4.563 -73.270 131.550 1.00 25.88 B	
05	MOTA	3670	CD	LYS	311		C
25	MOTA	3671	CE	LYS	311		C
	ATOM	3672	NZ	LYS	311		N
	MOTA	3673	С	LYS	311		C
	ATOM	3674	0	LYS	311		0
	ATOM	3675	N	LEU	312		N
30	MOTA	3676	CA	LEU	312		С
	MOTA	3677	CB	LEU	312		С
	MOTA	3678	CG	LEU	312		C
	MOTA	3679	CD1	LEU	312	7.304 -79.599 127.750 1.00 20.29 B	C
	MOTA	3680	CD2	LEU	312	6.853 -77.459 126.561 1.00 19.66 B	С
35	ATOM	3681	C	LEU	312	2.601 -78.075 127.029 1.00 20.37 B	С
	ATOM	3682	0	LEU	312	2.274 -78.074 125.840 1.00 19.79 B	0
	ATOM	3683	N	LEU	313	1.790 -78.513 127.989 1.00 19.32 B	N
	ATOM	3684	CA	LEU	313		C
	ATOM	3685	CB	LEU	313		С
40	ATOM	3686	CG	LEU	313		C
	ATOM	3687	CD1	LEU	313		С
	MOTA	3688		LEU	313		C
	ATOM	3689	С	LEU	313		C
	ATOM	3690	0	LEU	313		Ō
45	ATOM	3691	N	GLY	314		N
	ATOM	3692	CA	GLY	314		C
	ATOM	3693	C	GLY	314		C
	ATOM	3694	ō	GLY	314		Ö
	ATOM	3695	N	LEU	315		N
50	MOTA	3696	CA	LEU	315		C
50		3697	CB	LEU	315		C
	MOTA	3698	CG	LEU	315	3.491 -73.558 125.027 1.00 20.14 B	C C
	MOTA					A 000 72 670 125 004 1 00 22 42 5	<u> </u>
	MOTA	3699		LEU	315	4.998 -73.678 125.204 1.00 22.43 B	C
55	ATOM	3700		LEU	315	3.141 -72.341 124.174 1.00 20.16 B	C
33	ATOM	3701	C	LEU	315		C
	ATOM	3702		LEU	315		0
	ATOM	3703		LEU	316		N
	MOTA	3704	CA	LEU	316	0.140 -78.038 122.728 1.00 22.07 B	С

-233-

		2525	-		216	0 400 70 440 100 000 44 -	_
	MOTA	3705	CB	LEU	316	0.122 -79.442 123.333 1.00 22.61 B	C
	ATOM	3706		LEU	316	1.463 -80.171 123.415 1.00 25.13 B	С
	ATOM	3707	CD1		316	1.259 -81.562 123.994 1.00 25.21 B	C
E	MOTA	3708	CD2		316	2.073 -80.266 122.021 1.00 27.32 B	С
5	MOTA	3709	С	LEU	316	-1.286 -77.633 122.356 1.00 22.16 B	C
	MOTA	3710	0	LEU	316	-1.723 -77.853 121.225 1.00 21.15 B	0
	MOTA	3711	N	ALA	317	-1.998 -77.042 123.319 1.00 22.21 B	N
	MOTA	3712	CA	ALA	317	-3.364 -76.575 123.123 1.00 22.68 B	С
	ATOM	3713	CB	ALA	317	-4.034 -76.321 124.482 1.00 22.13 B	С
10	ATOM	3714	С	ALA	317	-3.380 -75.296 122.284 1.00 23.40 B	C
	ATOM	3715	0	ALA	317	-4.256 -75.115 121.437 1.00 22.48 B	0
	ATOM	3716	N	GLU	318	-2.422 -74.404 122.527 1.00 23.64 B	N
	ATOM	3717	CA	GLU	318	-2.347 -73.164 121.763 1.00 25.42 B	C
	ATOM	3718	СВ	GLU	318	-1.266 -72.242 122.325 1.00 27.16 B	Č
15	ATOM	3719	CG	GLU	318	-1.393 -70.797 121.859 1.00 32.13 B	Ċ
. •	ATOM	3720	CD	GLU	318	-0.190 -69.944 122.233 1.00 34.93 B	Č
	ATOM	3721		GLU	318	0.321 -70.093 123.362 1.00 37.73 B	ŏ
	ATOM	3722	OE2	GLU	318	0.239 -69.114 121.402 1.00 36.75 B	ŏ
	ATOM	3723	C	GLU	318	-2.036 -73.490 120.298 1.00 25.14 B	Č
20	ATOM	3724	ŏ	GLU	318	-2.557 -72.851 119.384 1.00 23.94 B	0
20		3725	-	LEU	319		
	MOTA		N				N
	ATOM	3726	CA	LEU	319	-0.814 -74.919 118.735 1.00 26.58 B	С
	MOTA	3727	CB	LEU	319	0.302 -75.961 118.818 1.00 27.06 B	С
25	ATOM	3728	CG	LEU	319	0.981 -76.399 117.524 1.00 28.14 B	C
25	ATOM	3729		LEU	319	1.450 -75.183 116.749 1.00 28.22 B	C
	MOTA	3730		LEU	319	2.156 -77.309 117.860 1.00 28.83 B	С
	MOTA	3731	С	LEU	319	-2.047 -75.508 118.036 1.00 26.66 B	C
	ATOM	3732	0	LEU	319	-2.200 -75.420 116.815 1.00 25.59 B	0
00	ATOM	3733	N	ARG	320	-2.926 -76.112 118.826 1.00 26.81 B	N
30	MOTA	3734	CA	ARG	320	-4.154 -76.671 118.298 1.00 27.51 B	С
	MOTA	3735	CB	ARG	320	-4.863 -77.471 119.388 1.00 30.21 B	C
	ATOM	3736	CG	ARG	320	-6.022 -78.298 118.892 1.00 34.14 B	C
	MOTA	3737	CD	ARG	320	-5.573 -79.252 117.808 1.00 37.44 B	C
~=	MOTA	3738	NE	ARG	320	-6.606 -80.233 117.500 1.00 41.15 B	N
35	MOTA	3739	CZ	ARG	320	-6.749 -81.403 118.118 1.00 42.64 B	C
	MOTA	3740	NH1	ARG	320	-5.919 -81.762 119.093 1.00 43.92 B	N
	MOTA	3741	NH2	ARG	320	-7.728 -82.222 117.755 1.00 43.56 B	N
	MOTA	3742	C	ARG	320	-5.022 -75.496 117.837 1.00 26.59 B	C
	MOTA	3743	0	ARG	320	-5.648 -75.551 116.781 1.00 26.01 B	0
40	ATOM	3744	N	SER	321	-5.055 -74.430 118.635 1.00 25.46 B	N
	MOTA	3745	CA	SER	321	-5.822 -73.235 118.283 1.00 25.37 B	C
	ATOM	3746	CB	SER	321	-5.676 -72.150 119.356 1.00 25.01 B	С
	ATOM	3747	OG	SER	321	-6.252 -72.562 120.577 1.00 28.59 B	0
	MOTA	3748	С	SER	321	-5.310 -72.681 116.964 1.00 24.05 B	C
45	MOTA	3749	0	SER	321	-6.090 -72.294 116.097 1.00 23.58 B	0
	MOTA	3750	N	ILE	322	-3.988 -72.636 116.834 1.00 23.19 B	
	ATOM	3751	CA	ILE	322	-3.339 -72.136 115.632 1.00 23.73 B	
	ATOM	3752	СВ	ILE	322	-1.800 -72.171 115.794 1.00 24.44 B	
	MOTA	3753	CG2		322	-1.115 -71.875 114.454 1.00 23.92 B	
50	MOTA	3754	CG1		322	-1.381 -71.170 116.878 1.00 24.48 B	
	ATOM	3755	CD1		322	0.068 -71.277 117.301 1.00 25.71 B	
	ATOM	3756	C	ILE	322	-3.759 -72.963 114.418 1.00 23.91 B	
	ATOM	3757	Ö	ILE	322	-4.004 -72.418 113.342 1.00 23.08 B	
	ATOM	3758	N	ASN	323	-3.853 -74.276 114.601 1.00 24.23 B	
55	ATOM	3759	CA	ASN	323	-4.258 -75.172 113.525 1.00 26.82 B	
55				ASN	323	-4.286 -76.617 114.033 1.00 29.48 B	
	ATOM	3760	CB				
	ATOM	3761	CG	ASN	323		_
	MOTA	3762	נעט	. ASN	323	-4.426 -78.796 113.058 1.00 32.81 B	0

-234-

	ATOM	3763	ND2	ASN	323	-3.386	-77.208	111.846	1.00 34.14	В	N
	ATOM	3764	С	ASN	323		-74.764		1.00 27.38	В	Ċ
	ATOM	3765	0	ASN	323		-74.546		1.00 26.41	В	ō
	ATOM	3766	N	GLU	324			113.959	1.00 27.46	В	N
5	ATOM	3767	CA	GLU	324		-74.246	113.612	1.00 28.72	В	C
	ATOM	3768	СВ	GLU	324		-74.253		1.00 30.37	В	Č
	ATOM	3769	CG	GLU	324		-75.615		1.00 34.56	В	č
	ATOM	3770	CD	GLU	324		-75.585		1.00 37.51	В	Č
	ATOM	3771	OE1		324		-74.660	117.598	1.00 38.60	В	ō
10	ATOM	3772	OE2		324		-76.492		1.00 39.78	В	ŏ
	ATOM	3773	C	GLU	324		-72.846		1.00 27.55	В	Ċ
	ATOM	3774	0	GLU	324		-72.574		1.00 28.12	В	ō
	ATOM	3775	N	ALA	325		-71.959	113.512	1.00 25.61	В	N
	ATOM	3776	CA	ALA	325		-70.607		1.00 24.75	В	c
15	ATOM	3777	СВ	ALA	325		-69.763	113.852	1.00 25.33	В	Ċ
	ATOM	3778	C	ALA	325		-70.642	111.539	1.00 24.31	В	Č
	ATOM	3779	Ō	ALA	325		-69.793		1.00 24.70	В	ŏ
	ATOM	3780	N	TYR	326		-71.613	111.223	1.00 23.49	В	N
	MOTA	3781	CA	TYR	326		-71.763		1.00 23.05	В	C
20	ATOM	3782	CB	TYR	326		-72.958		1.00 21.78	В	Č
	MOTA	3783	CG	TYR	326		-72.576		1.00 20.85	В	č
	ATOM	3784	CD1		326		-71.844		1.00 20.27	В	Č
	ATOM	3785	CE1	TYR	326		-71.492		1.00 19.55	В	Č
	MOTA	3786	CD2	TYR	326		-72.945		1.00 20.45	В	Ċ
25	MOTA	3787	CE2	TYR	326		-72.596		1.00 19.56	В	Ċ
	MOTA	3788	CZ	TYR	326				1.00 19.09	В	С
	ATOM	3789	OH	TYR	326		-71.527		1.00 17.47	В	0
	ATOM	3790	С	TYR	326		-72.001		1.00 23.60	В	C
	MOTA	3791	0	TYR	326			107.876	1.00 23.00	В	0
30	MOTA	3792	N	GLY	327	-7.304	-72.862	109.425	1.00 23.42	В	N
	MOTA	3793	CA	GLY	327			108.669	1.00 24.68	В	C
	ATOM	3794	C	GLY	327	-9.318	-71.936	108.354	1.00 26.46	В	C
	ATOM	3795	0	GLY	327	-9.790	-71.773	107.234	1.00 25.91	В	0
	MOTA	3796	N	TYR	328	-9.491	-71.056	109.337	1.00 27.71	В	N
35	MOTA	3797	CA	TYR	328	-10.246	-69.831	109.111	1.00 29.17	В	C
	MOTA	3798	CB	TYR	328	-10.460	-69.077	110.432	1.00 30.61	В	C
	ATOM	3799	CG	TYR	328	-11.094	-67.711	110.253	1.00 32.99	В	C
	MOTA	3800	CD1	TYR	328	-10.335	-66.618	109.826	1.00 33.59	В	C
	MOTA	3801	CE1	TYR	328	-10.921	-65.381	109.578	1.00 33.86	В	С
40	ATOM	3802	CD2	TYR	328	-12.465	-67.524	110.437	1.00 34.14	В	С
	ATOM	3803	CE2	TYR	328	-13.065	-66.281	110.191	1.00 34.54	В	C
	MOTA	3804	CZ	TYR	328		-65.219		1.00 35.00	В	C
	ATOM	3805	OH	TYR	328			109.484	1.00 35.60	В	0
	ATOM	3806	С	TYR	328	-9.528	-68.936	108.099	1.00 29.11	В	C
45	MOTA	3807	0	TYR	328			107.252	1.00 28.12	В	0
	ATOM	3808	N	GLN	329			108.188	1.00 29.12	В	N
	MOTA	3809	CA	GLN	329			107.272	1.00 29.08	В	С
	MOTA	3810	CB	GLN	329			107.652	1.00 27.70	В	C
	MOTA	3811	CG	GLN	329			109.016	1.00 26.09	В	C
50	MOTA	3812	CD	GLN	329			109.079	1.00 25.68	В	C
	MOTA	3813	OE1		329			109.898	1.00 26.08	В	0
	MOTA	3814	NE2		329			108.209	1.00 24.01	В	N
	MOTA	3815	С	GLN	329			105.812	1.00 30.18	В	C
	MOTA	3816	0	GLN	329			104.932	1.00 29.17	В	0
55	MOTA	3817	N	ILE	330			105.561	1.00 31.28	В	N
	MOTA	3818	CA	ILE	330			104.206	1.00 34.04	В	C
	MOTA	3819	CB	ILE	330			104.140	1.00 35.02	В	С
	MOTA	3820	CG2	LLE	330	-7.869	-72.640	105.155	1.00 36.98	В	C

-235-

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	MOTA	3821	CG1		330		-72.370		1.00 36.93		C
	MOTA	3822		ILE	330		-73.776		1.00 37.83		C
	ATOM	3823	_	ILE	330		-70.233		1.00 34.84		C
_	MOTA	3824		ILE	330		-70.200		1.00 33.41		0
5	MOTA	3825		GLN	331	-10.064			1.00 36.52	_	N
	MOTA	3826		GLN	331	-11.435			1.00 39.11		C
	MOTA	3827		GLN	331	-12.414			1.00 41.52		C
	MOTA	3828		GLN	331	-12.738			1.00 45.93	В	C
	ATOM	3829	CD	GLN	331	-11.691			1.00 48.62	В	С
10	ATOM	3830	OE1	GLN	331	-11.565	-73.397	106.400	1.00 50.00	В	0
	ATOM	3831	NE2	GLN	331	-10.934	-73.793	104.278	1.00 50.06	В	N
	ATOM	3832	С	GLN	331	-11.856	-68.651	103.741	1.00 38.77	В	C
	ATOM	3833	0	GLN	331	-12.764			1.00 39.36	В	0
	ATOM	3834	N	HIS	332	-11.188	-67.719	104.408	1.00 38.40	В	N
15	MOTA	3835	CA	HIS	332	-11.552	-66.316	104.290	1.00 38.62	В	С
	MOTA	3836	CB	HIS	332	-11.752	-65.742	105.690	1.00 40.74	В	C
	ATOM	3837	CG	HIS	332	-12.988	-66.250	106.368	1.00 43.93	В	С
	ATOM	3838	CD2		332	-13.214	-67.384	107.075	1.00 44.81	В	С
	ATOM	3839	ND1		332		-65.591		1.00 44.67	В	N
20	ATOM	3840	CE1		332		-66.296		1.00 45.90	В	С
	ATOM	3841	-	HIS	332		-67.389	107.419	1.00 45.60	В	N
	ATOM	3842	C	HIS	332		-65.418		1.00 37.56	В	C
	ATOM	3843	ŏ	HIS	332		-64.287		1.00 36.45	В	0
	ATOM	3844	N	ILE	333		-65.915		1.00 36.43	В	N
25	ATOM	3845	CA	ILE	333			102.369	1.00 35.55	В	C
	ATOM	3846	CB	ILE	333			103.194	1.00 35.40	В	C
	ATOM	3847	CG2		333	-	-64.090		1.00 35.90	В	Ċ
	ATOM	3848		ILE	333			104.392	1.00 35.38	В	Ċ
	MOTA	3849	CD1		333			105.558	1.00 35.02	В	Ċ
30	ATOM	3850	C	ILE	333			101.097	1.00 35.05	В	Č
00	MOTA	3851	Ö	ILE	333			101.108	1.00 34.80	В	ŏ
	ATOM	3852	N	GLN	334			100.003	1.00 33.98	В	N
	ATOM	3853	CA	GLN	334		-66.072		1.00 33.55	В	C
	ATOM	3854	CB	GLN	334		-65.284		1.00 34.76	В	Č
35	ATOM	3855	CG	GLN	334		-65.984		1.00 37.74	В	Ċ
55		3856	CD	GLN	334		-65.145		1.00 37.74	В	Ċ
	MOTA		OE1		334		-64.335		1.00 40.63	В	ŏ
	MOTA	3857	NE2		334		-65.329		1.00 41.05	В	N
	ATOM	3858					-66.101		1.00 41.03	В	C
40	MOTA	3859	С	GLN	334		-65.106		1.00 31.83	В	Ö
40	ATOM	3860	0	GLN	334		-67.250		1.00 30.79	В	N
	ATOM	3861	N	GLY	335		-67.356		1.00 30.05	В	C
	MOTA	3862	CA	GLY	335				1.00 30.05	В	_
	MOTA	3863	C	GLY	335		-68.065				C O
AE	MOTA	3864	0	GLY	335		-68.703		1.00 28.90	В	
45	MOTA	3865	N	LEU	336		-67.964		1.00 28.28	В	И
	ATOM	3866		LEU	336			100.772	1.00 28.50	В	C
	MOTA	3867		LEU	336		-68.352		1.00 26.88	В	C
	MOTA	3868		LEU	336			102.775	1.00 26.76	В	C
50	MOTA	3869		LEU	336			104.198	1.00 25.90	В	C
50	MOTA	3870		2 LEU	336			102.781	1.00 26.43	В	C
	MOTA	3871		LEU	336			7 100.561		В	C
	MOTA	3872		LEU	336			100.761		В	0
	MOTA	3873		SER	337			100.149		В	N
	MOTA	3874		SER	337		-72.208			В	C
55	MOTA	3875		SER	337		2 -72.63			В	C
	ATOM	3876		SER	337		L -72.034			В	
	MOTA	3877		SER			L -72.70				-
	MOTA	3878	0	SER	337	-3.374	4 -73.869	9 98.931	1.00 30.50	В	0

-236-

	MOTA	3879	N	ALA	338		-71.828	97.996	1.00 29.75	В	N
	MOTA	3880	CA	ALA	338		-72.188	96.983	1.00 30.35	В	C
	ATOM	3881	CB	ALA	338	-2.134	-71.015	96.043	1.00 29.79	В	С
_	MOTA	3882	C	ALA	338		-72.615	97.615	1.00 30.54	В	C
5	MOTA	3883	0	ALA	338		-73.408	97.037	1.00 31.26	В	0
	MOTA	3884	N	MET	339	-0.736	-72.082	98.796	1.00 30.39	В	N
	MOTA	3885	CA	MET	339	0.499	-72.427	99.494	1.00 31.18	В	C
	MOTA	3886	СВ	MET	339	0.906	-71.293	100.443	1.00 28.38	В	С
40	ATOM	3887	CG	MET	339		-70.061	99.719	1.00 27.58	В	C
10	ATOM	3888	SD	MET	339	1.777	-68.662	100:804	1.00 25.78	В	S
	ATOM	3889	CE	MET	339	0.137	-67.932	100.914	1.00 26.72	В	C
	ATOM	3890	С	MET	339	0.399	-73.742	100.267	1.00 33.29	В	C
	MOTA	3891	0	MET	339		-74.253		1.00 32.44	В	0
	MOTA	3892	N	MET	340	-0.810	-74.283	100.389	1.00 36.51	В	N
15	MOTA	3893	CA	MET	340	-0.993	-75.546	101.091	1.00 41.83	В	C
	MOTA	3894	CB	MET	340	-2.462	-75.740	101.480	1.00 43.44	В	C
	MOTA	3895	ÇG	MET	340	-2.713	-76.879	102.469	1.00 46.96	В	C
	MOTA	3896	SD	MET	340	-1.738	-76.795	104.011	1.00 50.06	В	S
	MOTA	3897	CE	MET	340	-1.302	-78.542	104.259	1.00 49.89	В	C
20	MOTA	3898	C	MET	340	-0.533	-76.639	100.126	1.00 44.42	В	C
	MOTA	3899	0	MET	340	-1.034	-76.737	99.008	1.00 43.85	В	0
	MOTA	3900	N	PRO	341	0.441	-77.463	100.556	1.00 47.61	В	N
	ATOM	3901	CD	PRO	341	0.791	-77.444	101.990	1.00 48.17	В	С
	MOTA	3902	CA	PRO	341	1.115	-78.593	99.902	1.00 50.66	В	C
25	MOTA	3903	CB	PRO	341	1.434	-79.506	101.076	1.00 49.85	В	C
	ATOM	3904	CG	PRO	341	1.857	-78.525	102.094	1.00 48.96	В	C
	MOTA	3905	С	PRO	341	0.470	-79.352	98.734	1.00 53.61	В	C
	ATOM	3906	0	PRO	341	1.190	-79.959	97.932	1.00 53.85	В	0
	ATOM	3907	N	LEU	342	-0.860	-79.329	98.640	1.00 56.59	В	N
30	ATOM	3908	CA	LEU	342	-1.595	-80.017	97.575	1.00 59.91	В	C
	MOTA	3909	CB	LEU	342	-0.835	-79.921	96.241	1.00 59.68	В	C
	MOTA	3910	CG	LEU	342	-1.238	-80.824	95.070	1.00 59.94	В	C
	ATOM	3911	CD1	LEU	342	-0.926	-80.135	93.752	1.00 59.43	В	C
	MOTA	3912	CD2	LEU	342	-0.506	-82.154	95.171	1.00 59.60	В	C
35	MOTA	3913	С	LEU	342	-1.845	-81.475	97.949	1.00 62.30	В	C
	ATOM	3914	0	LEU	342	-2.944	-81.997	97.749	1.00 62.71	В	0
	MOTA	3915	N	LEU	343	-0.821	-82.126	98.493	1.00 64.97	В	N
	MOTA	3916	CA	LEU	343	-0.923	-83.516	98.922	1.00 67.52	В	C
	MOTA	3917	CB	LEU	343	0.379	-83.961	99.600	1.00 67.63	В	C
40	MOTA	3918	CG	LEU	343	1.710	-83.566	98.956	1.00 67.80	В	C
	MOTA	3919	CD1	LEU	343	2.846	-84.029	99.847	1.00 67.88	В	C
	MOTA	3920	CD2	LEU	343	1.828	-84.171	97.567	1.00 67.91	В	С
	MOTA	3921	C	LEU	343		-83.599		1.00 68.96	В	С
	MOTA	3922	0	LEU	343	-3.019	-84.362	99.758	1.00 68.99	В	0
45	MOTA	3923	N	GLN	344	-1.950	-82.794	100.985	1.00 70.83	В	N
	MOTA	3924	CA	GLN	344	-2.944	-82.737	102.048	1.00 72.62	В	С
	MOTA	3925	CB	GLN	344	-2.496	-81.747	103.128	1.00 72.48	В	C
	MOTA	3926	CG	GLN	344	-1.098	-82.006	103.663	1.00 72.55	В	C
	ATOM	3927	CD	GLN	344	-1.003	-83.308	104.428	1.00 72.59	В	С
50	MOTA	3928	OE1	GLN	344	-1.517	-83.424	105.540	1.00 72.49	В	0
	MOTA	3929	NE2		344			103.832	1.00 72.52	В	N
	MOTA	3930	C	GLN	344			101.495	1.00 73.91	В	C
	MOTA	3931	0	GLN	344	-5.312	-82.970	101.740	1.00 74.16	В	0
	MOTA	3932	N	GLU	345			100.745	1.00 75.31	В	N
55	MOTA	3933	CA	GLU	345			100.166	1.00 76.49	В	С
	MOTA	3934	СВ	GLU	345			101.288	1.00 77.05	В	C
	ATOM	3935	CG	GLU	345			100.846	1.00 77.78	В	C
	MOTA	3936		GLU	345			102.005	1.00 78.25	В	

-237-

	ATOM	3937	OE1	_	345	-8.867	-80.087	102.987	1.00 78.37	В	0
	MOTA	3938	OE2		345		-78.184	101.937	1.00 78.57	В	0
	MOTA	3939	С	GLU	345	-5.258	-79.557	99.193	1.00 76.87	В	C
_	MOTA	3940	0	GLU	345	-5.484	-79.744	97.978	1.00 77.22	В	0
5	ATOM	3941	OXT	GLU	345	-4.802	-78.490	99.657	1.00 77.25	В	0
	TER	3942		GLU	345					В	
	MOTA	3943	CB	PRO	103	17.203	-24.177	122.780	1.00 92.75	C	C
	ATOM	3944	CG	PRO	103	15.916	-24.008	121.973	1.00 93.01	С	С
	ATOM	3945	C	PRO	103	16.591	-26.001	124.396	1.00 92.31	C	C
10	MOTA	3946	0	PRO	103	15.433	-26.410	124.489	1.00 92.32	C	0
	MOTA	3947	N	PRO	103	16.430	-26.298	121.930	1.00 92.88	C	N
	MOTA	3948	CD	PRO	103			121.064	1.00 93.06	C	C
	MOTA	3949	CA	PRO	103			123.033	1.00 92.61	C	C
	ATOM	3950	N	VAL	104			125.450	1.00 91.79	Č	N
15	ATOM	3951	CA	VAL	104			126.812	1.00 91.07	C	C
	ATOM	3952	CB	VAL	104			127.462	1.00 91.34	C	C
	ATOM	3953	CG1	VAL	104			126.766	1.00 91.17	C	C
	MOTA	3954	CG2	VAL	104			127.359	1.00 91.18	Ċ	C
	MOTA	3955	С	VAL	104			127.691	1.00 90.40	Č	Ċ
20	ATOM	3956	0	VAL	104			128.310	1.00 90.36	Č	ō
	ATOM	3957	N	GLN	105			127.742	1.00 89.40	Č	N
	MOTA	3958	CA	GLN	105			128.519	1.00 88.14	C	С
	MOTA	3959	CB	GLN	105			127.879	1.00 88.78	Č	Ċ
	ATOM	3960	CG	GLN	105			126.631	1.00 89.73	C	C
25	ATOM	3961	CD	GLN	105			125.438	1.00 90.20	Ċ	Ċ
	MOTA	3962	OE1	GLN	105			125.406	1.00 90.33	Č	Ō
	MOTA	3963	NE2	GLN	105			124.450	1.00 90.48	Č	N
	ATOM	3964	С	GLN	105			129.975	1.00 86.74	C	C
	MOTA	3965	0	GLN	105			130.372	1.00 87.04	C	0
30	ATOM	3966	N	LEU	106			130.763	1.00 84.58	C	N
	ATOM	3967	CA	LEU	106	14.831	-22.211	132.176	1.00 82.19	C	C
	ATOM	3968	CB	LEU	106			132.907	1.00 82.41	C	C
	MOTA	3969	CG	LEU	106			134.361	1.00 82.27	C	C
	MOTA	3970	CD1	LEU	106	13.961	-24.027	134.458	1.00 82.05	C	C
35	ATOM	3971	CD2	LEU	106	16.356	-24.611	134.870	1.00 82.24	C	C
	ATOM	3972	С	LEU	106	14.920	-20.833	132.834	1.00 80.39	С	C
	ATOM	3973	0	LEU	106	15.976	-20.432	133.322	1.00 80.25	С	0
	ATOM	3974	N	SER	107	13.798	-20.118	132.833	1.00 78.12	C	N
	MOTA	3975	CA	SER	107	13.698	-18.781	133.413	1.00 75.92	С	C
40	ATOM	3976	CB	SER	107	12.229	-18.437	133.670	1.00 75.50	C	С
	ATOM	3977	OG	SER	107	12.106	-17.218	134.377	1.00 74.70	С	0
	ATOM	3978	С	SER	107	14.484	-18.613	134.708	1.00 74.75	C	С
	ATOM	3979	0	SER	107	14.622	-19.552	135.491	1.00 74.59	C	0
	ATOM	3980	N	LYS	108	14.998	-17.405	134.927	1.00 73.23	C	N
45	ATOM	3981	CA	LYS	108	15.761	-17.109	136.134	1.00 71.45	C	C
	ATOM	3982	CB	LYS	108	16.580	-15.825	135.954	1.00 71.64	C	C
	MOTA	3983	CG	LYS	108	15.752	-14.553	135.829	1.00 71.83	С	C
	MOTA	3984	CD	LYS	108	16.621	-13.317	135.598	1.00 72.24	C	C
	MOTA	3985	CE	LYS	108	17.070	-13.171	134.142	1.00 72.27	С	C
50	ATOM	3986	NZ	LYS	108	18.040	-14.211	133.689	1.00 72.65	С	N
	MOTA	3987	С	LYS	108	14.828	-16.966	137.334	1.00 70.06	С	C
	MOTA	3988	0	LYS	108			138.475	1.00 69.77	C	0
	MOTA	3989	N	GLU	109	13.572	-16.611	. 137.074	1.00 68.53	С	N
	MOTA	3990	CA	GLU	109	12.589	-16.460	138.139	1.00 66.79	С	С
55	MOTA	3991	CB	GLU	109	11.342	-15.742	137.627	1.00 67.72	С	С
	MOTA	3992	CG	GLU	109	10.312	-15.496	138.709	1.00 69.22	С	C
	MOTA	3993	CD	GLU	109			138.212	1.00 70.31	С	C
	ATOM	3994	OE1	GLU	109	9.308	-13.573	137.740	1.00 70.89	С	0

-238-

	MOTA	3995	OE2		109			138.297	1.00 71.04	C	0
	MOTA	3996	C	GLU	109			138.678	1.00 64.99	C	C
	MOTA	3997	0	GLU	109			139.887	1.00 64.83	С	0
_	MOTA	3998	N	GLN	110			137.782	1.00 62.56	C	N
5	MOTA	3999	CA	GLN	110			138.220	1.00 60.51	C	C
	MOTA	4000	CB	GLN	110			137.066	1.00 60.12	C	C
	ATOM	4001	CG	GLN	110			135.821	1.00 59.34	C	C
	MOTA	4002	CD	GLN	110			134.607	1.00 58.88	C	C
40	MOTA	4003	OE1		110			133.587	1.00 58.96	C	0
10	MOTA	4004	NE2	GLN	110			134.709	1.00 58.28	C	N
	MOTA	4005	C	GLN	110			138.830	1.00 59.45	С	C
	MOTA	4006	0	GLN	110			139.561	1.00 59.18	C	0
	MOTA	4007	N	GLU	111			138.538	1.00 57.98	C	N
45	ATOM	4008	CA	GLU	111			139.139	1.00 56.65	C	С
15	MOTA	4009	CB	GLU	111			138.501	1.00 57.99	C	C
	ATOM	4010	CG	GLU	111			137.131	1.00 59.95	C	C
	MOTA	4011	CD	GLU	111			136.885	1.00 61.39	C	С
	ATOM	4012		GLU	111			137.121 136.453	1.00 61.89	C	0
20	ATOM	4013		GLU	111			140.613	1.00 61.84	C	c
20	ATOM	4014	C	GLU	111				1.00 54.63	Ç	0
	MOTA	4015	0	GLU	111			141.478	1.00 54.15 1.00 52.67	C	И
	ATOM	4016 4017	N	GLU	112 112			140.881	1.00 52.67	C	C
	MOTA	4017	CA CB	GLU GLU	112			142.209	1.00 52.04	C	C
25	MOTA	4018	CG	GLU	112			143.560	1.00 53.83	c	c
25	MOTA MOTA	4019	CD	GLU	112			144.552	1.00 55.38	Ç	Č
	ATOM	4020		GLU	112			144.575	1.00 56.05	C	Ö
	ATOM	4021		GLU	112			145.324	1.00 56.06	c	ŏ
	ATOM	4023	C	GLU	112			143.022	1.00 48.98	Č	č
30	ATOM	4024		GLU	112			144.149	1.00 48.54	Č	ŏ
-	ATOM	4025	N	LEU	113			142.409	1.00 46.59	Č	Ŋ
	ATOM	4026	CA	LEU	113			143.013	1.00 43.90	Č	C
	ATOM	4027	СВ	LEU	113			142.030	1.00 43.46	č	Ċ
	ATOM	4028	CG	LEU	113			142.419	1.00 42.93	C	C
35	ATOM	4029		LEU	113			143.685	1.00 41.97	С	C
	ATOM	4030		LEU	113			141.272	1.00 42.66	C	C
	ATOM	4031	С	LEU	113	12.225	-22.181	L 143.396	1.00 42.33	С	С
	ATOM	4032	0	LEU	113	12.042	-22.672	2 144.502	1.00 41.47	С	0
	ATOM	4033	N	ILE	114	12.978	-22.768	3 142.476	1.00 41.11	C	N
40	MOTA	4034	CA	ILE	114	13.640	-24.031	1 142.766	1.00 40.20	С	C
	MOTA	4035	CB	ILE	114			9 141.521	1.00 39.72	С	C
	MOTA	4036	CG2	ILE	114			5 141.902	1.00 39.64	-	_
	MOTA	4037	CG1	LILE	114			7 140.458	1.00 40.14	С	С
	MOTA	4038	CD	LILE	114			5 139.226	1.00 39.70	C	
45	ATOM	4039	С	ILE	114			8 143.914	1.00 39.98		
	ATOM	4040	0	ILE	114			4 144.782	1.00 39.82		
	ATOM	4041	N	ARG	115			5 143.916			
	ATOM	4042		ARG	115			2 144.956			C
	ATOM	4043		ARG	115			6 144.670			
50	ATOM	4044		ARG	115			5 145.596			
	MOTA	4045		ARG	115			5 146.953			
	ATOM	4046		ARG	115			4 146.880			
	MOTA	4047		ARG	115			2 147.901			
EC	MOTA	4048		1 ARG	115			2 149.086			
55	ATOM	4049		2 ARG	115			5 147.739			
	ATOM	4050		ARG	115			0 146.315			
	ATOM	4051		ARG	115			9 147.260			
	ATOM	4052	N	THR	116	14.552	2 -21.63	9 146.401	1.00 36.28	C	N

-239-

	MOTA	4053	CA	THR	116		-21.512		1.00 34.60	С	С
	ATOM	4054	СВ	THR	116		-20.439		1.00 35.71	C	C
	MOTA	4055	OG1		116		-20.351		1.00 37.91	C	0
_	ATOM	4056		THR	116		-20.776		1.00 37.42	C	C
5	MOTA	4057	C	THR	116		-22.864	148.098	1.00 32.61	С	С
	ATOM	4058	0	THR	116		-23.189	149.287	1.00 31.75	C	0
	ATOM	4059	N	LEU	117		-23.660		1.00 30.08	C	N
	ATOM	4060	CA	LEU	117		-24.971		1.00 28.36	C	С
40	MOTA	4061	CB	LEU	117		-25.614		1.00 26.76	С	С
10	MOTA	4062	CG	LEU	117		-24.967		1.00 25.75	C	С
	ATOM	4063		LEU	117	9.678	-25.739	144.568	1.00 25.12	C	C
	ATOM	4064	CD2	LEU	117	9.114	-24.940	146.855	1.00 24.24	C	С
	ATOM	4065	C	LEU	117	13.233	-25.904	148.030	1.00 28.17	C	C
	ATOM	4066	0	LEU	117	13.052	-26.608	149.022	1.00 27.39	C	0
15	MOTA	4067	N	LEU	118	14.370	-25.908	147.344	1.00 27.82	C	N
	ATOM	4068	CA	LEU	118	15.498	-26.751	147.726	1.00 27.94	C	C
	MOTA	4069	CB	LEU	118	16.605	-26.639	146.673	1.00 28.74	C	С
	ATOM	4070	CG	LEU	118		-27.775		1.00 30.12	C	C
	ATOM	4071		LEU	118		-28.136		1.00 30.71	Č	Ċ
20	ATOM	4072		LEU	118		-27.350		1.00 31.14	Č	Č
	ATOM	4073	C	LEU	118		-26.383		1.00 27.07	č	Č
	ATOM	4074	ŏ	LEU	118		-27.255		1.00 26.71	Č	ŏ
	ATOM	4075	N	GLY	119			149.366	1.00 26.49	č	Ň
	ATOM	4076	CA	GLY	119			150.655	1.00 26.44	Č	C
25	ATOM	4077	C	GLY	119			151.782	1.00 26.03	Č	C
	ATOM	4078	Ö	GLY	119			152.714	1.00 25.94	Č	Ö
	ATOM	4079	N	ALA	120			151.694	1.00 25.49	C	N
	ATOM	4080	CA	ALA	120			152.707	1.00 24.69	C	C
	MOTA	4081	CB	ALA	120			152.707	1.00 24.69		C
30	MOTA	4082	C	ALA	120			152.329	1.00 24.34	C	C
00	MOTA	4082	Ö	ALA	120			152.858		C	
	ATOM	4084	N	HIS	121				1.00 23.29	C	0
	MOTA							151.730	1.00 23.87	C	N
		4085	CA	HIS	121			151.733	1.00 23.41	C	C
35	ATOM	4086	CB	HIS	121			150.302	1.00 23.48	C	C
33	MOTA	4087	CG	HIS	121			150.197	1.00 23.06	C	C
	MOTA	4088		HIS	121			150.383	1.00 22.98	C	С
	ATOM	4089		HIS	121			149.890	1.00 24.73	C	N
	ATOM	4090		HIS	121			149.890	1.00 24.22	С	С
40	MOTA	4091		HIS	121			150.187	1.00 24.19	C	N
40	MOTA	4092	С	HIS	121	14.743		152.394	1.00 23.45	C	C
	MOTA	4093	0	HIS	121	14.648		153.230	1.00 22.84	С	0
	MOTA	4094	N	THR	122			152.018	1.00 23.17	C	N
	MOTA	4095	CA	THR	122			152.591	1.00 23.53	С	C
45	MOTA	4096	CB	THR	122			151.918	1.00 23.68	C	C
45	MOTA	4097		THR	122	18.483		150.560	1.00 23.80	C	0
	MOTA	4098		THR	122	19.675		152.657	1.00 23.99	C	С
	MOTA	4099	С	THR	122			154.106	1.00 23.12	C	C
	MOTA	4100	0	THR	122			154.872	1.00 22.20	C	0
	ATOM	4101	N	ARG	123	16.826		154.535	1.00 22.95	C	N
50	MOTA	4102	CA	ARG	123	16.843		155.954	1.00 23.76	С	C
	MOTA	4103	CB	ARG	123			156.131	1.00 25.69	C	С
	ATOM	4104	CG	ARG	123	16.825	-25.737	157.549	1.00 28.57	С	C
	MOTA	4105	CD	ARG	123	16.329	-24.291	157.692	1.00 30.95	С	С
	ATOM	4106	NE	ARG	123	16.999	-23.365	156.775	1.00 33.62	C	N
55	ATOM	4107	CZ	ARG	123			156.996	1.00 34.51	C	C
	ATOM	4108		L ARG	123			158.111	1.00 33.79	C	N
	ATOM	4109		2 ARG	123			156.095	1.00 34.90	C	N
	MOTA	4110		ARG	123			156.819	1.00 22.89	Ċ	C
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-240-

	ATOM	4111	0	ARG	123		-28.945		1.00 22.11	C	0
	MOTA	4112	N	HIS	124	14.651	-28.824	156.298	1.00 21.71	С	N
	MOTA	4113	CA	HIS	124	13.618	-29.483	157.101	1.00 21.10	С	С
	ATOM	4114	CB	HIS	124	12.399	-28.565	157.175	1.00 20.20	С	С
5	ATOM	4115	CG	HIS	124	12.701	-27.207	157.718	1.00 19.38	С	С
	MOTA	4116	CD2	HIS	124	13.214	-26.818	158.909	1.00 17.97	С	С
	ATOM	4117	ND1	HIS	124	12.473	-26.050	157.002	1.00 19.43	C	N
	MOTA	4118	CE1	HIS	124	12.832	-25.008	157.731	1.00 18.44	С	C
	MOTA	4119	NE2	HIS	124	13.285	-25.447	158.892	1.00 18.55	С	N
10	ATOM	4120	С	HIS	124	13.108	-30.888	156.790	1.00 21.31	С	C
	ATOM	4121	0	HIS	124	12.579	-31.555	157.684	1.00 20.78	С	0
	ATOM	4122	N	MET	125	13.253	-31.352	155.555	1.00 21.02	C	N
	ATOM	4123	CA	MET	125			155.210	1.00 21.61	С	C
	ATOM	4124	СВ	MET	125	11.498	-32.478	154.301	1.00 22.63	C	C
15	ATOM	4125	CG	MET	125		-31.555		1.00 24.18	C	C
	ATOM	4126	SD	MET	125			154.075	1.00 26.74	C	S
	ATOM	4127	CE	MET	125			152.446	1.00 26.67	C	С
	ATOM	4128	C	MET	125			154.572	1.00 20.49	C	С
	MOTA	4129	Ó	MET	125	13.567	-34.860	154.856	1.00 19.83	C	0
20	MOTA	4130	N	GLY	126			153.706	1.00 20.13	С	N
	MOTA	4131	CA	GLY	126			153.015	1.00 19.93	C	C
	MOTA	4132	C	GLY	126			153.840	1.00 20.19	C	C
	ATOM	4133	0	GLY	126	16.140	-36.333	153.376	1.00 19.39	C	0
	ATOM	4134	N	THR	127			155.064	1.00 20.00	C	N
25	ATOM	4135	CA	THR	127			155.918	1.00 20.76	C	C
	ATOM	4136	СВ	THR	127			156.155	1.00 20.73	C	C
	ATOM	4137	OG1		127			156.638	1.00 20.90	C	0
	ATOM	4138	CG2		127			154.850	1.00 19.98	Ċ	C
	MOTA	4139	C	THR	127			157.267	1.00 20.55	C	C
30	MOTA	4140	Ō	THR	127			158.245	1.00 19.57	C	0
	ATOM	4141	N	MET	128			157.318	1.00 20.36	C	N
	ATOM	4142	CA	MET	128			158.566	1.00 20.82	C	C
	ATOM	4143	СВ	MET	128			158.419	1.00 21.34	C	C
	ATOM	4144	CG	MET	128			157.523	1.00 21.05	C	С
35	ATOM	4145	SD	MET	128			157.462	1.00 20.70	С	S
_	ATOM	4146	CE	MET	128			156.233	1.00 21.69	C	C
	ATOM	4147	C	MET	128			159.019	1.00 20.76	C	C
	ATOM	4148	0	MET	128			160.207	1.00 19.74	С	0
	ATOM	4149	N	PHE	129			158.071	1.00 21.12	C	N
40	ATOM	4150	CA	PHE	129			158.386	1.00 21.43	С	С
	ATOM	4151	СВ	PHE	129			157.089	1.00 23.16	C	C
	ATOM	4152	CG	PHE	129	15.407	-40.543	156.385	1.00 25.47	C	С
	ATOM	4153	CD1	PHE	129	16.397	-41.413	156.827	1.00 25.73	С	С
	MOTA	4154		PHE	129	15.677	-39.719	155.298	1.00 26.68	С	С
45	MOTA	4155		PHE	129	17.637	-41.465	156.200	1.00 28.33	С	С
	ATOM	4156	CE2	PHE	129	16.913	-39.758	3 154.661	1.00 27.60	С	С
	ATOM	4157	CZ	PHE	129	17.897	-40.632	2 155.112	1.00 28.66	С	С
	ATOM	4158	C	PHE	129	15.229	-40.150	159.300	1.00 20.85	С	С
	MOTA	4159	0	PHE	129	15.070	-41.163	3 159.983	1.00 19.76	C	0
50	ATOM	4160	N	GLU	130	16.363	-39.450	159.314	1.00 20.93	С	N
	ATOM	4161	CA	GLU	130			160.153	1.00 22.74	С	C
	ATOM	4162	СВ	GLU	130			5 159.875	1.00 24.78	С	C
	ATOM	4163	CG	GLU	130			6 158.446		C	C
	ATOM	4164		GLU	130			4 158.231		C	C
55	ATOM	4165		l GLU	130			9 159.051		C	0
	MOTA	4166		2 GLU	130			6 157.236		С	
	ATOM	4167		GLU	130			3 161.637		C	
	ATOM	4168		GLU	130			7 162.445		С	

-241-

	ATOM	4169	N	GLN	131	16.152	-39.001	161.989	1.00 20.13	C	N
	ATOM	4170	CA	GLN	131	15.770	-38.843	163.382	1.00 20.44	C	C
	ATOM	4171	CB	GLN	131	15.199	-37.442	163.622	1.00 20.12	С	C
	MOTA	4172	CG	GLN	131		-36.305		1.00 22.04	C	С
5	ATOM	4173	CD	GLN	131		-36.478		1.00 22.44	Č	C
	ATOM	4174	OE1		131			165.156	1.00 20.89	Č	ŏ
	ATOM	4175	NE2		131		-36.347		1.00 21.74	Ċ	N
	ATOM	4176	C	GLN	131		-39.880	163.878	1.00 20.14	č	c
	ATOM	4177	ŏ	GLN	131		-39.947		1.00 19.21	c	ŏ
10	ATOM	4178	N	PHE	132		-	162.970	1.00 19.21	C	N
10	ATOM	4179	CA	PHE	132			163.360			
	ATOM	4180	CB	PHE	132				1.00 18.44	C	C
								162.162	1.00 17.81	C	C
	ATOM	4181	CG	PHE	132			161.104	1.00 18.33	C	C
15	MOTA	4182	CD1		132			161.286	1.00 18.03	C	C
15	ATOM	4183	CD2	PHE	132			159.920	1.00 17.90	C	C
	ATOM	4184	CE1		132			160.299	1.00 18.71	C	C
	MOTA	4185	CE2	PHE	132				1.00 18.59	C	C
	MOTA	4186	CZ	PHE	132			159.125	1.00 18.77	C	С
	MOTA	4187	C	PHE	132			164.478	1.00 18.64	C	С
20	MOTA	4188	0	PHE	132	13.022	-43.061	165.353	1.00 16.29	C	0
	MOTA	4189	N	VAL	133	15.081	-42.866	164.446	1.00 18.83	C	N
	MOTA	4190	CA	VAL	133	15.699	-43.714	165.450	1.00 19.85	C	Ċ
	MOTA	4191	CB	VAL	133	17.195	-43.995	165.102	1.00 20.35	C	C
	MOTA	4192	CG1	VAL	133	18.012	-42.709	165.177	1.00 19.58	С	С
25	ATOM	4193	CG2	VAL	133	17.758	-45.072	166.034	1.00 20.81	C	C
	MOTA	4194	С	VAL	133	15.589	-43.124	166.857	1.00 20.00	С	C
	ATOM	4195	0	VAL	133	15.698	-43.847	167.841	1.00 20.01	С	0
	ATOM	4196	N	GLN	134			166.957	1.00 20.18	C	N
	ATOM	4197	CA	GLN	134			168.261	1.00 19.68	Ċ	C
30	MOTA	4198	СВ	GLN	134			168.187	1.00 20.98	Č	Č
	ATOM	4199	CG	GLN	134			167.598	1.00 21.75	č	č
	ATOM	4200	CD	GLN	134		-40.182		1.00 24.09	č	č
	ATOM	4201		GLN	134			167.982	1.00 25.24	Č	ō
	ATOM	4202	NE2		134			169.577	1.00 23.24	č	N
35	ATOM	4203	C	GLN	134			168.847	1.00 25.20	Č	C
v	ATOM	4204	ō	GLN	134			169.909	1.00 18.53	Č	o
	ATOM	4205	N	PHE	135			168.178	1.00 17.76	Č	N
	ATOM	4206	CA	PHE	135			168.656	1.00 17.70	C	C
	ATOM	4207	CB	PHE	135			167.599	1.00 17.30	C	C
40	ATOM	4208	CG	PHE	135			167.467	1.00 15.94	C	C
40	ATOM	4209		PHE	135			168.406	1.00 15.94	C	C
	ATOM	4210		PHE	135			166.432	1.00 15.05	C	
	ATOM	4211		PHE	135			168.323			C
		4211	CE2						1.00 16.31	C	C
45	ATOM				135			166.337	1.00 15.93	C	C
45	ATOM	4213	CZ	PHE	135			167.288	1.00 15.48	C	C
	ATOM	4214	C	PHE	135			169.072	1.00 17.74	C	C
	ATOM	4215	0	PHE	135			168.587	1.00 16.28	C	0
	ATOM	4216	N	ARG	136			169.982	1.00 18.46	C	N
5 0	MOTA	4217	CA	ARG	136			170.522	1.00 20.06	С	C
50	MOTA	4218	СВ	ARG	136			7 171.516	1.00 20.96	C	C
	MOTA	4219	CG	ARG	136			172.580	1.00 24.90	С	С
	MOTA	4220	CD	ARG	136			2 173.505	1.00 26.50	С	C
	MOTA	4221	NE	ARG	136			3 172.903	1.00 27.43	С	N
	MOTA	4222	CZ	ARG	136			3 173.598	1.00 27.58	С	С
55	MOTA	4223		ARG	136			7 174.903	1.00 27.65	С	N
	MOTA	4224	NH2	ARG	136	6.124	-42.262	2 173.001	1.00 27.78	C	N
	ATOM	4225	С	ARG	136	11.095	-46.386	5 169.489	1.00 19.43	С	С
	MOTA	4226		ARG	136	10.042	-47.008	3 169.585	1.00 20.16	C	0
		_		_							

-242-

	MOTA	4227		PRO	137		-46.614		1.00 18.91		N
	MOTA	4228		PRO	137		-46.014		1.00 18.50		C
	MOTA	4229	_	PRO	137		-47.637		1.00 18.39		C
_	MOTA	4230		PRO	137			166.406	1.00 18.19		C
5	MOTA	4231		PRO	137			167.190	1.00 18.43		C
	MOTA	4232		PRO	137			168.119	1.00 18.32		C
	MOTA	4233		PRO	137			168.849	1.00 17.61		0
	ATOM	4234		PRO	138			167.845	1.00 18.18		N
40	MOTA	4235		PRO	138			167.165	1.00 18.09		C
10	MOTA	4236	CA	PRO	138			168.407	1.00 18.53	C	C
	ATOM	4237	CB	PRO	138			167.905	1.00 19.26		C
	ATOM	4238	CG	PRO	138			167.784	1.00 20.92		C
	MOTA	4239	С	PRO	138			167.851	1.00 18.85		С
4.5	MOTA	4240	0	PRO	138			166.767	1.00 17.83		0
15	MOTA	4241	N	ALA	139			168.585	1.00 18.83		N
	MOTA	4242	CA	ALA	139			168.170	1.00 19.23	С	С
	MOTA	4243	CB	ALA	139			169.249	1.00 19.24		С
	MOTA	4244	С	ALA	139			166.811	1.00 20.00	C	C
	MOTA	4245	0	ALA	139			166.090	1.00 19.18	C	0
20	MOTA	4246	N	HIS	140			166.448	1.00 19.64	C	N
	MOTA	4247	CA	HIS	140			165.180	1.00 20.90	C	C
	MOTA	4248	СВ	HIS	140			165.073	1.00 19.67	C	C
	ATOM	4249	CG	HIS	140			164.690	1.00 20.46	С	C
05	MOTA	4250	CD2		140			163.508	1.00 20.20	C	С
25	MOTA	4251		HIS	140			165.577	1.00 19.33	C	N
	MOTA	4252		HIS	140			164.959	1.00 20.25	C	C
	ATOM	4253		HIS	140			163.704	1.00 20.65	C	N
	MOTA	4254	С	HIS	140			163.927	1.00 21.31	С	C
20	MOTA	4255	0	HIS	140			162.827	1.00 21.71	C	0
30	MOTA	4256	N	LEU	141			164.092	1.00 21.64	C	N
	MOTA	4257	CA	LEU	141			162.964	1.00 22.55	C	С
	ATOM	4258	CB	LEU	141			163.223	1.00 21.20	С	C
	MOTA	4259	CG	LEU	141			163.475	1.00 21.22	C	C
25	MOTA	4260		LEU	141			163.714	1.00 19.35	C	C
35	ATOM	4261		LEU	141			162.274	1.00 20.05	C	C
	ATOM	4262	C	LEU	141			162.672	1.00 23.75	C	C
	ATOM	4263	0	LEU	141			161.647	1.00 23.76	C	0
	ATOM	4264	N	PHE	142			163.560	1.00 24.92	C	N
40	ATOM	4265	CA	PHE	142			163.377	1.00 27.83	C	C
40	MOTA	4266	CB	PHE	142			164.733	1.00 26.48	C	C
	ATOM	4267	CG	PHE	142			165.535	1.00 26.04	C	C
	ATOM	4268		PHE	142			166.508	1.00 26.71	C	
	ATOM	4269		PHE	142			165.340	1.00 25.71	C	C
45	ATOM	4270		PHE	142			167.283	1.00 26.31	C	C
40	ATOM	4271		PHE	142			166.107	1.00 25.93	C	C
	ATOM	4272	CZ	PHE	142			167.080	1.00 24.84	C	C
	MOTA	4273	C	PHE	142			3 162.428	1.00 29.94	C	C
	ATOM	4274	0	PHE	142			3 162.376		C	0
50	MOTA	4275		ILE	143			161.704		C	N
50	ATOM	4276		ILE	143			5 160.756			C
	MOTA	4277		ILE	143			3 161.497 3 160 510		C	C
	MOTA	4278		ILE	143			9 160.519		C	C
	MOTA	4279		ILE	143			162.632		C	C
55	MOTA	4280		ILE	143			2 162.192 9 150 657			C
JJ	MOTA	4281		ILE	143			9 159.657 8 159 493			C
	MOTA	4282		ILE				8 158.483 9 160 030			O
	MOTA	4283		HIS	144			9 160.030 7 150 002			N
	MOTA	4284	CA	HIS	144	17.425	7 -20.08	7 159.082	1.00 39.85	C	С

-243-

	3 0004	4005	00		2.4.4	10 100	C7 430	150 001		_	_
	ATOM	4285	СВ	HIS	144		-57.439		1.00 42.16	C	C
	MOTA	4286	CG	HIS	144		-58.290		1.00 44.99	C	C
	ATOM	4287	CD2	HIS	144	16.240	-58.062	157.112	1.00 45.85	C	С
	ATOM	4288	ND1	HIS	144	17.800	-59.550	157.460	1.00 46.31	С	N
5	ATOM	4289	CE1		144		-60.061		1.00 46.80	c	Ċ
-	ATOM	4290	NE2		144	16.008	-59.178		1.00 46.60		
										C	N
	ATOM	4291	С	HIS	144		-56.302		1.00 39.44	C	C
	ATOM	4292	0	HIS	144			160.809	1.00 38.57	C	0
	MOTA	4293	N	HIS	145	15.026	-55.812	159.075	1.00 39.00	C	N
10	ATOM	4294	CA	HIS	145	13.693	-55.972	159.615	1.00 39.08	С	C
	MOTA	4295	CB	HIS	145	12.639	-55.528	158.596	1.00 38.43	C	С
	ATOM	4296	CG	HIS	145		-55.408	159.171	1.00 38.37	Č	Ċ
	ATOM	4297		HIS	145		-54.322	159.566	1.00 37.79	C	c
	ATOM	4298		HIS	145			159.433	1.00 37.79		
15										C	N
13	MOTA	4299		HIS	145			159.963	1.00 37.12	C	C
	MOTA	4300		HIS	145			160.056	1.00 37.13	C	N
	MOTA	4301	С	HIS	145	13.486	-57.436	159.988	1.00 39.30	C	C
	ATOM	4302	0	HIS	145	13.828	-58.343	159.223	1.00 38.89	C	0
	MOTA	4303	N	GLN	146	12.949	-57.650	161.185	1.00 38.87	C	N
20	ATOM	4304	CA	GLN	146	12,670	-58.984	161.690	1.00 38.47	C	C
	ATOM	4305	CB	GLN	146			163.036	1.00 39.68	Č	c
	ATOM	4306	CG	GLN	146	14.769		162.991	1.00 33.08	C	c
	ATOM	4307	CD								
				GLN	146			164.389	1.00 43.84	C	C
25	MOTA	4308	OE1		146			165.116	1.00 45.31	C	0
25	MOTA	4309	NE2		146			164.791	1.00 44.12	C	N
	MOTA	4310	С	GLN	146	11.178	-59.107	161.887	1.00 37.20	C	С
	MOTA	4311	0	GLN	146	10.515	-58.161	162.303	1.00 37.37	C	0
	ATOM	4312	N	PRO	147	10.624	-60.284	161.600	1.00 35.99	C	N
	ATOM	4313	CD	PRO	147			161.151	1.00 35.90	C	C
30	ATOM	4314	CA	PRO	147			161.788	1.00 34.04	č	Ċ
	ATOM	4315	CB	PRO	147			161.700	1.00 34.54		
										C	С
	ATOM	4316	CG	PRO	147			161.570	1.00 35.92	C	C
	MOTA	4317	C	PRO	147			163.249	1.00 32.25	C	C
25	MOTA	4318	0	PRO	147			164.166	1.00 31.73	C	0
35	MOTA	4319	N	LEU	148	7.754	-59.406	163.463	1.00 29.88	C	N
	MOTA	4320	CA	LEU	148	7.265	-59.167	164.811	1.00 26.83	C	С
	ATOM	4321	CB	LEU	148	6.273	-58.001	164.808	1.00 27.33	C	C
	ATOM	4322	CG	LEU	148			166.142	1.00 28.42	C	C
	ATOM	4323		LEU	148			167.091	1.00 28.52	c	č
40	ATOM	4324		LEU	148		-56.420		1.00 28.07	C	C
	ATOM	4325	C	LEU	148			165.156	1.00 28.07		
										C	C
	ATOM	4326	0	LEU	148			164.344	1.00 22.45	C	0
	MOTA	4327	N	PRO	149			166.342	1.00 22.72	C	N
4 ==	MOTA	4328	CD	PRO	149			167.337	1.00 21.82	С	C
45	ATOM	4329	CA	PRO	149	6.171	-62.301	166.704	1.00 21.92	C	С
	MOTA	4330	CB	PRO	149	6.704	-62.579	168.107	1.00 20.94	C	C
	ATOM	4331	CG	PRO	149	8.085	-61.986	168.051	1.00 22.25	С	C
	ATOM	4332	C	PRO	149			166.667	1.00 21.18	Ċ	C
	ATOM	4333	ŏ	PRO	149			166.859	1.00 21.31	Č	Ö
50	ATOM	4334	N	THR	150			166.427	1.00 20.81	c	
30											N
	ATOM	4335	CA	THR	150			166.352	1.00 20.80	C	С
	MOTA	4336	CB	THR	150			166.233	1.00 19.51	С	С
	MOTA	4337	OG1		150	2.553	-65.453	164.951	1.00 17.95	С	0
	MOTA	4338	CG2	THR	150	0.649	-65.107	166.404	1.00 19.20	С	С
55	ATOM	4339	С	THR				167.532	1.00 21.88	С	C
	ATOM	4340	0	THR	150			167.336	1.00 21.66	C	ō
	ATOM	4341	N	LEU	151			168.751	1.00 21.61	č	N
	ATOM	4342	CA	LEU	151			169.931	1.00 21.32	Č	C
	OH	4J42	CA	TEU	101	1.52/	-02.003	, 103.331	1.00 21.32	C	C

-244-

	MOTA	4343	-	LEU	151		796 170.964	1.00 20.79		C
	MOTA	4344		LEU	151		995 170.548	1.00 20.54		С
	MOTA	4345	CD1		151		025 171.675	1.00 20.72		C
_	MOTA	4346	CD2		151	-0.926 -64.		1.00 19.30		C
5	MOTA	4347	C	LEU	151		455 170.567	1.00 21.12		C
	ATOM	4348	0	LEU	151		012 171.641	1.00 21.25	C	0
	MOTA	4349	N	ALA	152		916 169.908	1.00 19.97	C	N
	MOTA	4350	CA	ALA	152	3.918 -59.	751 170.433	1.00 19.76	C	C
	ATOM	4351	CB	ALA	152	5.205 -59.	516 169.649	1.00 18.98	С	С
10	MOTA	4352	С	ALA	152	3.022 -58.	506 170.365	1.00 19.64	C	С
	MOTA	4353	0	ALA	152	2.337 -58.	267 169.370	1.00 18.40	С	0
	MOTA	4354	N	PRO	153		705 171.439	1.00 19.90	С	N
	MOTA	4355	CD	PRO	153	3.636 -57.	923 172.754	1.00 20.17	С	C
	MOTA	4356	CA	PRO	153	2.177 -56.	495 171.446	1.00 20.12	C	C
15	ATOM	4357	CB	PRO	153	2.503 -55.	865 172.801	1.00 20.62	C	С
	ATOM	4358	CG	PRO	153	2.784 -57.	067 173.669	1.00 20.46	C	C
	ATOM	4359	С	PRO	153	2.555 -55.	573 170.286	1.00 20.10	C	С
	ATOM	4360	0	PRO	153	3.734 -55.	405 169.989	1.00 19.34	C	0
	MOTA	4361	N	VAL	154	1.558 -54.	986 169.626	1.00 21.19	С	N
20	MOTA	4362	CA	VAL	154	1.834 -54.	071 168.522	1.00 22.10	С	С
	MOTA	4363	CB	VAL	154	0.763 -54.	191 167.388	1.00 23.65	C	С
	ATOM	4364	CG1	VAL	154	-0.590 -53.	693 167.869	1.00 24.74	С	С
	MOTA	4365	CG2	VAL	154	1.201 -53.	395 166.172	1.00 24.89	С	С
	ATOM	4366	С	VAL	154	1.900 -52.	623 169.026	1.00 21.26	С	С
25	ATOM	4367	0	VAL	154		726 168.296	1.00 21.70	С	0
	ATOM	4368	N	LEU	155	1.516 -52.	408 170.284	1.00 20.70	C	N
	ATOM	4369	CA	LEU	155	1.529 -51.	075 170.902	1.00 19.78	C	С
	MOTA	4370	СВ	LEU	155		188 172.393	1.00 19.93	С	C
	ATOM	4371	CG	LEU	155		911 173.250	1.00 21.72	C	C
30	ATOM	4372		LEU	155		872 172.660	1.00 20.06	C	C
_	ATOM	4373	-	LEU	155		257 174.681	1.00 21.99	C	C
	ATOM	4374	C	LEU	155		304 170.726	1.00 18.83	C	C
	ATOM	4375	Ö	LEU	155		121 170.406	1.00 19.02	C	0
	ATOM	4376	N	PRO	156		954 170.942	1.00 18.50	C	N
35	ATOM	4377	CD	PRO	156		259 171.571	1.00 17.61	С	C
	ATOM	4378	CA	PRO	156		179 170.754	1.00 17.22	C	C
	MOTA	4379	СВ	PRO	156	-	.174 171.141	1.00 16.78	C	С
	ATOM	4380	CG	PRO	156		.011 172.205	1.00 17.22	C	C
	ATOM	4381	C	PRO	156	5.400 -49	.660 169.314	1.00 17.71	C	C
40	ATOM	4382	Ö	PRO	156		.539 169.093	1.00 16.22	C	0
. •	ATOM	4383	N	LEU	157		.479 168.342	1.00 16.66	C	N
	ATOM	4384	CA	LEU	157		.089 166.942	1.00 17.15	C	С
	ATOM	4385	СВ	LEU	157	4.726 -51	.267 166.019	1.00 15.68	С	С
	ATOM	4386	CG	LEU	157		.951 164.516	1.00 14.50	С	C
45	ATOM	4387		LEU	157		.381 164.153	1.00 12.24	C	C
	ATOM	4388		LEU	157		.203 163.714	1.00 11.45	С	C
	ATOM	4389	C	LEU	157		.932 166.688	1.00 16.47	C	C
	ATOM	4390	Ö	LEU	157		.971 166.016	1.00 16.30	C	0
	ATOM	4391	N	VAL	158		.039 167.229	1.00 16.36	Č	N
50	ATOM	4392		VAL	158		.003 167.088		C	C
•	ATOM	4393		VAL	158		.438 167.762		C	C
	ATOM	4394		L VAL	158		.291 167.732		Č	č
	ATOM	4395		2 VAL	158		.662 167.046		c	c
	ATOM	4396		VAL	158		.690 167.727		Č	c
55	ATOM	4397		VAL	158		.613 167.154		č	o
-	ATOM	4397		THR	159		.782 168.919		c	N
	ATOM	4399			159		.595 169.605		C	
									C	C
	MOTA	4400	CB	THR	159	4.045 -45	.956 170.976	1.00 10.34	C	C

-245-

	ATOM	4401	OG1		159		-46.585		1.00 15.26	C	0
	MOTA	4402		THR	159		-44.700		1.00 17.16	C	C
	MOTA	4403	С	THR	159	4.527	-44.930	168.755	1.00 16.11	C	C
_	MOTA	4404	0	THR	159	4.539	-43.710	168.602	1.00 17.45	C	0
5	MOTA	4405	N	HIS	160	5.426	-45.742	168.206	1.00 15.29	С	N
	ATOM	4406	CA	HIS	160	6.509	-45.257	167.351	1.00 14.74	C	C
	MOTA	4407	CB	HIS	160	7.397	-46.430	166.912	1.00 14.28	С	C
	MOTA	4408	CG	HIS	160	8.445	-46.055	165.905	1.00 13.23	Ç	C
	MOTA	4409	CD2	HIS	160	8.627	-46.444	164.620	1.00 13.10	C	С
10	MOTA	4410	ND1	HIS	160	9.462	-45.168	166.182	1.00 13.39	С	N
	MOTA	4411	CE1	HIS	160	10.228	-45.027	165.112	1.00 13.13	С	С
	MOTA	4412	NE2	HIS	160	9.744	-45.792	164.151	1.00 12.34	С	N
	MOTA	4413	С	HIS	160	5.961	-44.541	166.116	1.00 14.39	С	С
	ATOM	4414	0	HIS	160	6.435	-43.463	165.757	1.00 14.03	C	0
15	MOTA	4415	N	PHE	161		-45.144		1.00 14.40	С	N
	ATOM	4416	CA	PHE	161			164.280	1.00 15.29	C	C
,		4417	СВ	PHE	161		-45.472		1.00 15.35	C	Č
	ATOM	4418	CG	PHE	161		-46.510		1.00 17.07	Č	Č
	ATOM	4419	CD1		161			162.313	1.00 15.87	Ċ	č
20	ATOM	4420		PHE	161			162.199	1.00 17.11	Ċ	č
	ATOM	4421		PHE	161			161.432	1.00 17.22	Č	c
	ATOM	4422	-	PHE	161			161.308	1.00 18.15	Ċ	c
	ATOM	4423	CZ	PHE	161			160.923	1.00 17.06	Č	Č
	ATOM	4424	C	PHE	161			164.636	1.00 17.00	C	c
25	ATOM	4425	Ö	PHE	161			163.928	1.00 13.30	C	Ö
	ATOM	4426	N	ALA	162			165.732	1.00 15.09	C	Ŋ
	ATOM	4427	CA	ALA	162			166.153	1.00 15.09	C	C
	ATOM	4428	CB	ALA	162			167.440	1.00 15.95	c	C
										C	C
30	MOTA	4429	C	ALA	162			166.358	1.00 15.56		
30	ATOM	4430	0	ALA	162			165.986	1.00 15.40	C	0
	MOTA	4431	N	ASP	163			166.938	1.00 16.37	C	N
	ATOM	4432	CA	ASP	163			167.165	1.00 17.11	C	C
	ATOM	4433	CB	ASP	163			168.039	1.00 18.76	C	C
35	MOTA	4434	CG	ASP	163			169.518	1.00 19.80	c	C
33	ATOM	4435		ASP	163			170.303	1.00 20.29	C	0
	ATOM	4436		ASP	163			169.896	1.00 20.75	c	0
	ATOM	4437	C	ASP	163			165.879	1.00 16.41	C	C
	ATOM	4438	0	ASP	163			165.703	1.00 16.53	C	0
40	ATOM	4439	N	ILE	164			164.976	1.00 15.27	C	N
40	ATOM	4440	CA	ILE	164			163.747	1.00 14.57	C	C
	ATOM	4441	CB	ILE	164			163.018	1.00 14.61	C	C
	MOTA	4442		ILE	164				1.00 12.74	C	
	ATOM	4443		ILE	164			162.497	1.00 13.93	C	C
45	ATOM	4444		ILE	164			161.668	1.00 15.42	С	С
45	MOTA	4445	С	ILE	164			162.801	1.00 14.37	С	C
	MOTA	4446	0	ILE	164			162.025	1.00 13.76	C	0
	ATOM	4447	N	ASN	165			162.854	1.00 13.47	С	N
	ATOM	4448	CA	ASN	165			162.018	1.00 14.22	С	С
	MOTA	4449	CB	ASN	165			162.189	1.00 13.22	С	C
50	MOTA	4450	CG	ASN	165			161.424	1.00 13.80	C	С
	MOTA	4451	_	. ASN	165			1 160.545	1.00 13.34	С	0
	MOTA	4452	ND2	ASN	165			9 161.748	1.00 11.89	С	N
	MOTA	4453	C	ASN	165			162.453	1.00 13.40	С	С
	MOTA	4454		ASN	165			3 161.620		С	0
55	MOTA	4455		THR	166			2 163.764		С	N
	ATOM	4456		THR	166			164.302		C	C
	MOTA	4457		THR	166	3.359	-36.27	165.807		С	C
	MOTA	4458	OG1	THR	166			9 165.995		С	0

-246-

	MOTA	4459		THR	166		-34.869		1.00 14.52	С	C
	ATOM	4460	C	THR	166	4.968	-35.403	164.064	1.00 15.86	C	C
	ATOM	4461	0	THR	166		-34.223		1.00 16.48	C	0
_	MOTA	4462	N	PHE	167	6.124	-36.035	164.234	1.00 17.03	C	N
5	ATOM	4463	CA	PHE	167		-35.373		1.00 16.78	C	С
	ATOM	4464	CB	PHE	167		-36.363		1.00 17.79	С	C
	MOTA	4465	CG	PHE	167	9.869	-35.942	163.675	1.00 18.70	C	C
	ATOM	4466	CD1	PHE	167	10.606	-34.915	164.256	1.00 19.29	C	C
	ATOM	4467	CD2	PHE	167	10.392	-36.594	162.558	1.00 19.25	C	С
10	ATOM	4468	CE1	PHE	167	11.851	-34.545	163.734	1.00 19.64	С	С
	ATOM	4469	CE2	PHE	167			162.030	1.00 19.87	С	C
	ATOM	4470	CZ	PHE	167	12.365	-35.208	162.617	1.00 19.58	C	C
	ATOM	4471	С	PHE	167	7.429	-34.887	162.532	1.00 16.84	С	C
	MOTA	4472	0	PHE	167	7.805	-33.744	162.251	1.00 16.80	С	0
15	ATOM	4473	N	MET	168	7.033	-35.755	161.603	1.00 15.69	С	N
	MOTA	4474	CA	MET	168	7.023	-35.397	160.187	1.00 14.91	C	C
	ATOM	4475	CB	MET	168	6.661	-36.608	159.312	1.00 14.73	С	С
	ATOM	4476	CG	MET	168	7.782	-37.634	159.161	1.00 12.77	C	C
	MOTA	4477	SD	MET	168	7.419	-38.898	157.918	1.00 13.46	С	S
20	ATOM	4478	CE	MET	168	6.583	-40.139	158.891	1.00 9.89	C	С
	MOTA	4479	С	MET	168			159.890	1.00 15.70	C	C
	ATOM	4480	0	MET	168			159.097	1.00 13.88	C	0
	MOTA	4481	N	VAL	169			160.510	1.00 16.72	C	N
	ATOM	4482	CA	VAL	169	3.926	-33.202	160.303	1.00 17.84	Ċ	С
25	ATOM	4483	СВ	VAL	169			161.132	1.00 18.74	C	C
	ATOM	4484	CG1	VAL	169			161.111	1.00 16.96	C	C
	ATOM	4485	CG2	VAL	169			160.544	1.00 17.94	C	C
	ATOM	4486	C	VAL	169			160.694	1.00 18.62	C	Ċ
	ATOM	4487	O	VAL	169			159.954	1.00 18.14	Ċ	Ō
30	ATOM	4488	N	LEU	170			161.850	1.00 19.05	Č	N
	ATOM	4489	CA	LEU	170			162.284	1.00 18.80	Č	C
	MOTA	4490	CB	LEU	170			163.700	1.00 19.18	Č	C
	MOTA	4491	CG	LEU	170			164.808	1.00 20.13	C	C
	MOTA	4492	CD1	LEU	170			166.112	1.00 20.19	Č	Č
35	ATOM	4493		LEU	170			164.983	1.00 21.80	C	С
	MOTA	4494	С	LEU	170			161.297	1.00 19.15	C	C
	ATOM	4495	0	LEU	170			161.055	1.00 19.95	Č	ō
	ATOM	4496	N	GLN	171			160.718	1.00 18.11	Č	N
	ATOM	4497	CA	GLN	171			159.743	1.00 17.90	Č	C
40	ATOM	4498	СВ	GLN	171			159.382	1.00 17.69	C	C
	ATOM	4499	CG	GLN	171			160.501	1.00 19.25	Č	Č
	ATOM	4500	CD	GLN	171	11.383	-31.408	161.040	1.00 19.45	C	
	ATOM	4501		GLN	171			160.305	1.00 21.44	C	O
	ATOM	4502		GLN	171			162.328	1.00 19.42	C	N
45	MOTA	4503	C	GLN	171			158.458	1.00 17.82	C	С
	ATOM	4504	Ō	GLN	171			157.841	1.00 17.25	C	ō
	MOTA	4505	N	VAL	172			158.039	1.00 17.26	C	N
	MOTA	4506	CA	VAL	172			7 156.834	1.00 18.43	Ċ	C
	ATOM	4507	CB	VAL	172			156.376	1.00 18.66	C	Č
50	ATOM	4508		VAL	172			7 155.185	1.00 17.80	C	C
	ATOM	4509		VAL	172			3 155.967	1.00 18.65	С	C
	ATOM	4510	C	VAL	172			157.107	1.00 18.42	C	Č
	ATOM	4511	ŏ	VAL	172			3 156.264	1.00 18.24	Č	ō
	ATOM	4512		ILE	173			5 158.286	1.00 18.42	Č	N
55	ATOM	4513	CA	ILE	173			3 158.644			C
	ATOM	4514	СВ	ILE	173			160.090			C
	ATOM	4515		: ILE	173			160.550			c
	ATOM	4516		ILE	173			6 160.330 6 160.147			C
	011	-3-0					•	,		~	_

-247-

	MOTA	4517		ILE	173			161.559	1.00 18.69	С	С
	MOTA	4518	С	ILE	173			158.509	1.00 18.47	C	C
	MOTA	4519	0	ILE	173			157.856	1.00 17.88	C	0
_	MOTA	4520		LYS	174			159.103	1.00 17.67	С	N
5	MOTA	4521		LYS	174			159.025	1.00 18.85	C	C
	MOTA	4522		LYS	174			159.797	1.00 19.84	C	C
	MOTA	4523	CG	LYS	174			161.293	1.00 20.37	C	C
	MOTA	4524	CD	LYS	174			161.996	1.00 22.31	С	C
40	MOTA	4525	CE	LYS	174			162.080	1.00 24.43	С	С
10	MOTA	4526	NZ	LYS	174			162.841	1.00 27.02	C	N
	ATOM	4527	C	LYS	174			157.568	1.00 19.16	C	C
	ATOM	4528	0	LYS	174			157.194	1.00 18.69	C	0
	MOTA	4529	N	PHE	175			156.758	1.00 18.61	C	N
15	MOTA	4530	CA	PHE	175			155.342	1.00 18.87	C	C
15	ATOM	4531	CB	PHE	175			154.697	1.00 18.31	C	C
	MOTA	4532	CG	PHE PHE	175 175			153.190	1.00 18.11	C	C
	MOTA	4533 4534	_	PHE	175			152.485 152.478	1.00 16.75 1.00 17.31	C	C
	MOTA ATOM	4534		PHE	175 175			152.478	1.00 17.31	C	C
20	ATOM	4536		PHE	175			151.090	1.00 17.12	C	C
20	ATOM	4537	CZ	PHE	175 175			150.386	1.00 16.84	C	C
	ATOM	4538	C	PHE	175			154.619	1.00 10.17	C	C
	ATOM	4539	Ö	PHE	175			153.875	1.00 19.63	C	Ö
	ATOM	4540	N	THR	176			154.834	1.00 19.92	č	N
25	ATOM	4541	CA	THR	176			154.181	1.00 21.48	Č	c
	ATOM	4542	СВ	THR	176			154.427	1.00 21.69	č	Č
	ATOM	4543	OG1		176			155.833	1.00 22.61	Č	ō
	ATOM	4544	CG2		176			153.886	1.00 20.21	Ċ	Č
	ATOM	4545	C	THR	176			154.668	1.00 22.48	C	C
30	ATOM	4546	0	THR	176			153.896	1.00 22.19	C	0
	ATOM	4547	N	LYS	177	6.521	-22.938	155.946	1.00 22.93	C	N
	ATOM	4548	CA	LYS	177	6.742	-21.606	156.491	1.00 24.72	C	C
	MOTA	4549	CB	LYS	177	6.833	-21.662	158.018	1.00 25.60	С	C
	MOTA	4550	CG	LYS	177	5.447	-21.769	158.658	1.00 28.46	C	C
35	ATOM	4551	CD	LYS	177			160.169	1.00 28.76	С	C
	MOTA	4552	CE	LYS	177			160.754	1.00 28.66	C	C
	MOTA	4553	NZ	LYS	177			160.208	1.00 29.61	С	N
	MOTA	4554	С	LYS	177			155.900	1.00 24.56	C	C
40	MOTA	4555	0	LYS	177			155.971	1.00 23.75	C	0
40	ATOM	4556	N	ASP	178			155.313	1.00 24.31	C	N
	ATOM	4557	CA	ASP	178			154.684	1.00 25.00	C	C
	ATOM	4558	CB	ASP	178				1.00 24.90		
	ATOM	4559	CG	ASP	178			156.238	1.00 25.48	C	C
45	MOTA	4560		ASP	178			157.090	1.00 26.26	C	0
43	ATOM	4561		ASP	178			156.478	1.00 24.33 1.00 25.18	C	0
	ATOM	4562	C	ASP	178			153.199	1.00 25.18	C	C
	MOTA	4563	0	ASP	178 179			1 152.448 1 152.772	1.00 24.75	C	0
	ATOM ATOM	4564 4565	N CA	LEU	179			3 151.379	1.00 24.75	C	N C
50	ATOM	4566	CB	LEU	179			150.822	1.00 23.10	C	C
50	MOTA	4567	CG	LEU	179			150.822	1.00 23.10	č	C
	ATOM	4568		LEU	179			150.173	1.00 22.10	C	C
	ATOM	4569		LEU	179			5 150.213	1.00 20.84		c
	ATOM	4570	CD2	LEU	179			150.213			C
55	ATOM	4571	o	LEU	179			7 151.623			
-	ATOM	4572	N	PRO	180			5 1 50.776			
	ATOM	4573	CD	PRO	180			3 150.770 3 150.417			
	ATOM	4574	CA	PRO	180			5 150.427			
										_	_

-248-

	MOTA	4575	СВ	PRO	180	8.446 -16.102 149.771 1.00 25.45 C C	
	MOTA	4576	CG	PRO	180	9.757 -16.576 150.309 1.00 25.01 C C	
	MOTA	4577	С	PRO	180	6.062 -16.973 150.003 1.00 25.06 C C	
_	MOTA	4578	0	PRO	180	5.107 -16.419 150.543 1.00 24.75 C O	
5	ATOM	4579	N	VAL	181	5.937 -17.676 148.880 1.00 25.37 C N	
	MOTA	4580	CA	VAL	181	4.637 -17.808 148.218 1.00 26.24 C C	
	MOTA	4581	CB	VAL	181	4.743 -18.624 146.898 1.00 27.68 C C	
	MOTA	4582	CG1	VAL	181	5.515 -17.822 145.857 1.00 28.55 C C	
<u></u>	ATOM	4583	CG2	VAL	181	5.424 -19.971 147.151 1.00 28.30 C C	
10	ATOM	4584	C	VAL	181	3.566 -18.439 149.113 1.00 25.72 C C	
	MOTA	4585	0	VAL	181	2.384 -18.116 148.996 1.00 25.14 C O	
	ATOM	4586	N	PHE	182	3.981 -19.341 149.997 1.00 25.42 C N	
	MOTA	4587	CA	PHE	182	3.062 -19.988 150.933 1.00 25.66 C C	
	MOTA	4588	CB	PHE	182	3.737 -21.199 151.602 1.00 24.81 C C	
15	MOTA	4589	CG	PHE	182	2.859 -21.923 152.598 1.00 24.52 C C	
	MOTA	4590		PHE	182	1.909 -22.845 152.172 1.00 24.87 C C	
	MOTA	4591		PHE	182	2.991 -21.687 153.966 1.00 25.69 C C	
	ATOM	4592	_	PHE	182	1.103 -23.524 153.089 1.00 23.82 C C	
	ATOM	4593	CE2	PHE	182	2.185 -22.362 154.897 1.00 25.07 C C	
20	ATOM	4594	CZ	PHE	182	1.240 -23.282 154.452 1.00 24.45 C C	
	MOTA	4595	С	PHE	182	2.676 -18.971 152.006 1.00 25.40 C C	
	MOTA	4596	0	PHE	182	1.497 -18.796 152.311 1.00 24.95 C C	
	MOTA	4597	N	ARG	183	3.679 -18.303 152.575 1.00 25.82 C N	
	MOTA	4598	CA	ARG	183	3.450 -17.309 153.624 1.00 27.71 C	
25	MOTA	4599	CB	ARG	183	4.787 -16.809 154.191 1.00 26.21 C	3
	MOTA	4600	CG	ARG	183	5.521 -17.831 155.048 1.00 25.37 C	
	MOTA	4601	CD	ARG	183	4.739 -18.176 156.325 1.00 24.60 C	
	MOTA	4602	NE	ARG	183		1
	ATOM	4603	CZ	ARG	183		C
30	MOTA	4604		. ARG	183		N
	MOTA	4605		ARG	183		N
	MOTA	4606	С	ARG	183		C
	MOTA	4607	0	ARG	183		0
0.5	MOTA	4608	N	SER	184		N
35	MOTA	4609	CA	SER	184		C
	MOTA	4610	CB	SER	184		C
	MOTA	4611	OG	SER	184		0
	MOTA	4612	C	SER	184		C
40	MOTA	4613	0	SER	184		0
40	MOTA	4614		LEU	185		N C
	ATOM	4615		LEU	185		C
	MOTA	4616	-	LEU	185		C
	ATOM	4617		LEU	185		c
45	MOTA	4618		1 LEU	185		C
45	ATOM	4619		2 LEU	185	-2.142 -16.345 152.693 1.00 32.89 C	c
	ATOM	4620		LEU	185 185		ö
	ATOM	4621		LEU	186		N
	MOTA	4622		PRO	186		C
50	MOTA	4623			186		c
30	MOTA	4624			186	-5.564 -15.552 153.588 1.00 34.21 C	c
	ATOM	4625			186		c
	MOTA	4626			186		c
	ATOM	4627		PRO	186		o
55	MOTA	4628		PRO ILE	187		И
J	ATOM	4629			187		C
	MOTA	4630			187	-3.844 -17.417 158.594 1.00 38.59 C	c
	MOTA	4631			187	-3.717 -18.588 159.562 1.00 39.09 C	C
	MOTA	4632	z CG	2 ILE	TO/	-3.717 -10.300 133.302 1.00 33.03 C	_

-249-

	ATOM	4633	CG1		187			158.871	1.00 39.17	C	С
	ATOM	4634	CD1		187			158.653	1.00 39.06	C	C
	MOTA	4635	С	ILE	187			156.964	1.00 37.72	C	C
_	ATOM	4636	0	ILE	187			157.055	1.00 37.65	C	0
5	MOTA	4637	N	GLU	188			156.717	1.00 37.53	C	N
	MOTA	4638	CA	GLU	188			156.535	1.00 37.86	C	C
	ATOM	4639	CB	GLU	188			156.286	1.00 39.84	C	C
	MOTA	4640	CG	GLU	188	-8.424	-18.286	155.155	1.00 43.27	C	C
	ATOM	4641	CD	GLU	188	-8.379	-16.849	155.645	1.00 45.23	С	C
10	ATOM	4642	OE1		188	-7.596	-16.550	156.578	1.00 45.96	С	0
	ATOM	4643	OE2	GLU	188	-9.125	-16.015	155.084	1.00 46.68	C	0
	ATOM	4644	С	GLU	188	-6.558	-20.832	155.397	1.00 36.71	C	C
	ATOM	4645	0	GLU	188	-6.786	-22.041	155.487	1.00 35.74	C	0
	ATOM	4646	N	ASP	189	-5.977	-20.292	154.330	1.00 35.44	C	N
15	ATOM	4647	CA	ASP	189			153.199	1.00 34.24	C	C
	MOTA	4648	CB	ASP	189	-5.378	-20.255	151.946	1.00 35.42	C	C
	MOTA	4649	CG	ASP	189	-6.701	-19.753	151.380	1.00 36.94	C	C
	MOTA	4650	OD1	ASP	189	-6.722	-19.324	150.210	1.00 38.00	С	0
	MOTA	4651	QD2	ASP	189	-7.717	-19.781	152.105	1.00 38.31	С	0
20	ATOM	4652	C	ASP	189			153.503	1.00 32.76	C	С
	ATOM	4653	0	ASP	189	-4.089	-22.998	153.001	1.00 31.31	C	0
	ATOM	4654	N	GLN	190	-3.397	-21.311	154.313	1.00 31.50	C	N
	ATOM	4655	CA	GLN	190	-2.165	-21.995	154.694	1.00 31.34	C	C
	MOTA	4656	CB	GLN	190			155.565	1.00 31.81	C	C
25	MOTA	4657	CG	GLN	190	-0.838	-19.803	154.884	1.00 32.88	C	C
	MOTA	4658	CD	GLN	190	0.168	-19.006	155.699	1.00 33.88	C	C
	MOTA	4659	OE1	GLN	190	0.376	-17.816	155.452	1.00 35.31	C	0
	MOTA	4660	NE2	GLN	190	0.805	-19.658	156.663	1.00 32.82	C	N
	MOTA	4661	С	GLN	190	-2.569	-23.242	155.484	1.00 30.49	C	C
30	ATOM	4662	0	GLN	190	-2.039	-24.326	155.258	1.00 29.34	С	0
	MOTA	4663	N	ILE	191	-3.520	-23.070	156.402	1.00 30.50	C	N
	ATOM	4664	CA	ILE	191			157.227	1.00 30.60	C	C
	ATOM	4665	CB	ILE	191	-5.216	-23.701	158.133	1.00 31.67	С	C
	ATOM	4666	CG2		191	-5.683	-24.857	159.000	1.00 30.87	C	C
35	MOTA	4667		ILE	191			159.006	1.00 32.04	C	C
	ATOM	4668		ILE	191			159.995	1.00 33.57	С	C
	MOTA	4669	С	ILE	191			156.334	1.00 30.25	С	С
	MOTA	4670	0	ILE	191			156.476	1.00 29.94	C	0
4.0	ATOM	4671	N	SER	192			155.415	1.00 28.90	C	N
40	MOTA	4672	CA	SER	192			154.503	1.00 28.72	C	C
	MOTA	4673	CB	SER	192			153.644	1.00 28.55	C	С
	MOTA	4674	OG	SER	192			154.472	1.00 31.09		0
	MOTA	4675	C	SER	192			153.605	1.00 27.78	С	C
45	MOTA	4676	0	SER	192			153.420	1.00 27.73	C	0
45	MOTA	4677	N	LEU	193			153.033	1.00 26.80	C	N
	MOTA	4678	CA	LEU	193			152.168	1.00 26.77	С	C
	MOTA	4679	СВ	LEU	193			151.415	1.00 26.32	С	C
	MOTA	4680	CG	LEU	193			150.384	1.00 26.16	C	С
E 0	ATOM	4681		LEU	193			2 149.513	1.00 26.75	C	C
50	MOTA	4682		LEU	193			149.519	1.00 24.72	C	C
	MOTA	4683	C	LEU	193			152.952	1.00 26.50	C	C
	MOTA	4684	0	LEU	193			152.468	1.00 25.42	C	0
	MOTA	4685	N	LEU	194			154.159	1.00 26.75	C	N
	MOTA	4686	CA	LEU	194			5 154.991	1.00 27.59	C	C
55	MOTA	4687	CB	LEU	194			2 156.301	1.00 28.17	C	C
	MOTA	4688	CG	LEU	194			157.201			C
	MOTA	4689		LEU	194			156.797			C
	MOTA	4690	CD2	LEU	194	-0.018	-27.79	5 158.662	1.00 32.14	С	С

-250-

	MOTA	4691	C	LEU	194		-29.246		1.00 27.29	C	C
	MOTA	4692	_	LEU	194		-30.328		1.00 26.70	C	0
	MOTA	4693	N	LYS	195		-29.148		1.00 26.53	С	N
_	MOTA	4694		LYS	195		-30.327		1.00 27.06	С	C
5	MOTA	4695		LYS	195		-29.918		1.00 28.79	С	C
	MOTA	4696		LYS	195		-29.205		1.00 31.86	C	C
	ATOM	4697	CD	LYS	195		-28.898		1.00 34.00	C	C
	MOTA	4698	CE	LYS	195		-28.259		1.00 35.25	C	C
	ATOM	4699	NZ	LYS	195		-28.066		1.00 37.11	C	N
10	MOTA	4700	C	LYS	195			154.956	1.00 26.13	C	C
	MOTA	4701	0	LYS	195			155.048	1.00 26.21	С	0
	MOTA	4702	N	GLY	196			153.812	1.00 24.83	C	N
	MOTA	4703	CA	GLY	196			152.606	1.00 23.63	С	C
. –	MOTA	4704	С	GLY	196			151.969	1.00 22.89	C	C
15	MOTA	4705	0	GLY	196			151.306	1.00 21.84	С	0
	MOTA	4706	N	ALA	197			152.179	1.00 21.49	С	N
	MOTA	4707	CA	ALA	197			151.545	1.00 21.24	С	C
	MOTA	4708	CB	ALA	197			150.584	1.00 19.64	C	C
	MOTA	4709	C	ALA	197			152.421	1.00 20.04	C	C
20	MOTA	4710	0	ALA	197			151.905	1.00 19.54	С	0
	MOTA	4711	N	ALA	198			153.717	1.00 18.80	С	N
	MOTA	4712	CA	ALA	198			154.616	1.00 17.78	С	C
	MOTA	4713	CB	ALA	198			156.052	1.00 17.25	С	C
	MOTA	4714	C	ALA	198			154.448	1.00 17.03	C	C
25	MOTA	4715	0	ALA	198			154.304	1.00 16.38	C	0
	MOTA	4716	N	VAL	199			154.482	1.00 16.43	С	N
	MOTA	4717	CA	VAL	199			154.332	1.00 16.70		C
	MOTA	4718	CB	VAL	199			154.613	1.00 16.81		C
	MOTA	4719		VAL	199			154.262	1.00 17.35		С
30	MOTA	4720	CG2	VAL	199			156.093	1.00 16.94		C
	MOTA	4721	C	VAL	199			152.934	1.00 16.67		C
	MOTA	4722	0	VAL	199			152.778	1.00 15.71		0
	MOTA	4723	N	GLU	200			151.920	1.00 16.31		N
~=	MOTA	4724	CA	GLU	200			150.546	1.00 17.25		C
35	MOTA	4725	СВ	GLU	200			149.589	1.00 18.45		C
	MOTA	4726	CG	GLU	200			149.242	1.00 19.72		C
	MOTA	4727	CD	GLU	200			148.399	1.00 20.49		
	MOTA	4728	OE1		200			147.526	1.00 20.99		
40	MOTA	4729		GLU	200			148.601	1.00 21.11		
40	MOTA	4730	C	GLU	200			2 150.373	1.00 17.44		
	MOTA	4731	0	GLU	200			149.792	1.00 16.76		
	MOTA	4732		ILE	201			150.875	1.00 17.66	_	
	ATOM	4733		ILE	201			3 150.794			
45	MOTA	4734		ILE	201			5 151.458			
45	MOTA	4735		ILE	201			9 151.706			
	MOTA	4736		LILE	201			8 150.561			
	MOTA	4737		LILE	201			8 151.190			
	MOTA	4738		ILE	201			6 151.491			
ΕO	MOTA	4739		ILE	201			3 150.976			
50	ATOM	4740		CYS	202			0 152.669			
	MOTA	4741		CYS	202			2 153.417			
	ATOM	4742		CYS	202			1 154.752			
	ATOM	4743		CYS	202			4 155.941			
E E	MOTA	4744		CYS	202			5 152.632			
55	ATOM	4745		CYS	202			5 152.684			
	ATOM	4746		HIS	203			9 151.908			
	MOTA	4747			203			8 151.121			
	MOTA	4748	CB	HIS	203	4.229	9 -40.44	2 150.611	1.00 15.9	z C	: c

-251-

	MOTA	4749	CG H	IIS	203	3.524	-41.272	151.640	1.00 15.86	С	С
	MOTA	4750	CD2 H	IIS	203	2.354	-41.080	152.293	1.00 16.22	С	С
	MOTA	4751	ND1 H	IIS	203	4.057	-42.439	152.145	1.00 16.53	С	N
_	MOTA	4752	CE1 H	iis	203	3.246	-42.930	153.064	1.00 16.84	C	С
5	MOTA	4753	NE2 H	iis	203	2.205	-42.123	153.174	1.00 16.72	С	N
	ATOM	4754	C H	iis	203	6.472	-39.519	149.962	1.00 16.55	C	С
	MOTA	4755	O H	iis	203	7.305	-40.352	149.601	1.00 17.66	С	0
	MOTA	4756	N I	LE	204	6.347	-38.331	149.378	1.00 16.27	C	N
	MOTA	4757	CA I	[LE	204	7.219	-37.944	148.284	1.00 16.29	C	C
10	MOTA	4758	CB I	[LE	204	6.806	-36.571	147.704	1.00 16.08	С	С
	MOTA	4759	CG2 I	LLE	204	7.903	-36.055	146.764	1.00 16.01	C	C
	ATOM	4760	CG1 I	(LE	204	5.469	-36.708	146.956	1.00 14.17	C	C
	MOTA	4761	CD1 1	[LE	204	4.892	-35.396	146.483	1.00 13.55	С	C
	MOTA	4762	C 1	ILE	204	8.664	-37.875	148.798	1.00 17.25	C	С
15	MOTA	4763	0 1	ILE	204	9.586	-38.383	148.159	1.00 17.11	С	0
	MOTA	4764	N V	VAL	205	8.847	-37.248	149.956	1.00 17.08	С	N
	ATOM	4765	CA \	VAL	205	10.159	-37.121	150.577	1.00 18.01	C	C
	MOTA	4766	CB 1	VAL	205			151.819	1.00 17.13	C	C
	ATOM	4767	CG1 V	VAL	205	11.383	-36.276	152.608	1.00 16.96	С	С
20	ATOM	4768	CG2 V	VAL	205	9.820	-34.765	151.372	1.00 16.00	C	С
	ATOM	4769	C /	VAL	205	10.711	-38.486	150.991	1.00 18.51	C	C
	ATOM	4770		VAL	205			150.799	1.00 19.15	C	0
	ATOM	4771		LEU	206			151.562	1.00 19.05	C	N
	ATOM	4772		LEU	206			151.993	1.00 20.76	C	С
25	ATOM	4773	CB I	LEU	206			152.848	1.00 21.98	C	C
	MOTA	4774		LEU	206			154.371	1.00 24.68	C	C
	MOTA	4775	CD1	LEU	206			154.882	1.00 24.95	C	C
	MOTA	4776	CD2	LEU	206	7.964	-41.484	155.032	1.00 24.49	C	С
	MOTA	4777	C	LEU	206	10.590	-41.629	150.841	1.00 20.80	C	C
30	MOTA	4778	0 :	LEU	206	11.225	-42.668	151.055	1.00 20.84	C	0
	ATOM	4779		ASN	207			149.623	1.00 19.96	C	N
	MOTA	4780		ASN	207			148.479	1.00 20.57	C	C
	ATOM	4781		ASN	207			147.199	1.00 18.23	C	C
	MOTA	4782	CG .	ASN	207	9.915	-42.530	146.017	1.00 18.97	C	C
35	MOTA	4783	OD1	ASN	207	10.590	-42.259	145.024	1.00 18.39	C	0
	ATOM	4784	ND2	ASN	207			146.123	1.00 16.71	C	N
	ATOM	4785	C .	ASN	207	11.939	-42.452	148.280	1.00 20.94	С	С
	ATOM	4786	0	ASN	207	12.308	-43.563	147.885	1.00 20.03	С	0
	ATOM	4787	N	THR	208	12.797	-41.469	148.556	1.00 20.81	C	N
40	ATOM	4788	CA	THR	208	14.235	-41.682	148.403	1.00 22.30	C	С
	MOTA	4789	CB	THR	208	15.058	-40.375	148.528	1.00 22.75	C	С
	MOTA	4790	OG1	THR	208	14.576	-39.590	149.624	1.00 22.99	C	0
	MOTA	4791	CG2	THR	208	14.974	-39.583	147.239	1.00 25.40	C	С
	ATOM	4792	С	THR	208	14.811	-42.708	149.372	1.00 21.11	С	С
45	MOTA	4793	0	THR	208	15.935	-43.148	149.190	1.00 21.58	C	0
	MOTA	4794	N	THR	209	14.061	-43.095	150.400	1.00 20.44	C	N
	MOTA	4795	CA	THR	209	14.567	-44.120	151.308	1.00 20.16	С	С
	MOTA	4796	CB	THR	209	14.114	-43.896	152.773	1.00 21.00	C	С
	ATOM	4797	OG1	THR	209	12.733	-44.268	3 152.920	1.00 20.06	С	0
50	ATOM	4798	CG2	THR	209	14.310	-42.427	7 153.178	1.00 19.21	С	C
	ATOM	4799		THR	209	14.086	-45.511	150.869	1.00 20.37	C	C
	ATOM	4800		THR	209			3 151.402	1.00 19.73	С	0
	ATOM	4801		PHE	210			149.886	1.00 19.78	С	N
	ATOM	4802	CA	PHE	210			3 149.404	1.00 21.06	C	С
55	ATOM	4803	CB	PHE	210			148.552	1.00 20.74	С	C
	ATOM	4804		PHE	210			3 148.271	1.00 20.23	С	С
	MOTA	4805			210			L 149.303	1.00 20.70	С	
	MOTA	4806	CD2	PHE	210	10.392	-48.204	146.969	1.00 19.93	С	

-252-

	MOTA	4807	CE1		210	9.062	-49.491	149.045	1.00 21.07	С	C
	MOTA	4808		PHE	210		-49.310		1.00 19.80	С	C
	MOTA	4809		PHE	210		-49.955		1.00 20.40	C	C
_	MOTA	4810		PHE	210		-47.647		1.00 21.28	C	С
5	MOTA	4811		PHE	210		-47.186		1.00 20.88	С	0
	MOTA	4812		CYS	211		-48.892		1.00 22.28	С	N
	MOTA	4813		CYS	211		-49.802		1.00 24.70	C	C
	ATOM	4814		CYS	211		-50.656		1.00 25.33	C	C
40	MOTA	4815		CYS	211		-51.838		1.00 28.07	С	S
10	ATOM	4816		CYS	211		-50.694		1.00 25.31	С	C
	MOTA	4817		CYS	211		-51.533		1.00 24.53	С	0
	MOTA	4818		LEU	212			146.111	1.00 26.95	С	N
	ATOM	4819		LEU	212			145.142	1.00 29.54	C	C
15	ATOM	4820		LEU	212			143.724	1.00 29.30	С	С
15	ATOM	4821		LEU	212			143.324	1.00 30.74	С	C
	ATOM	4822	CD1		212			142.004	1.00 30.10	C	C
	ATOM	4823	CD2		212			143.211	1.00 28.92	C	C
	ATOM	4824		LEU	212			145.298	1.00 30.81	C	C
20	ATOM	4825	0	LEU	212			145.277	1.00 30.78	C	0
20	MOTA	4826	N	GLN	213			145.469	1.00 31.69	C	N
	ATOM	4827	CA	GLN	213			145.616	1.00 33.12	C	C
	ATOM ATOM	4828	CB	GLN	213			145.725	1.00 35.87	C	C
	_	4829	CG CD	GLN	213 213			145.991	1.00 39.28	C	C
25	MOTA MOTA	4830 4831		GLN GLN	213			146.143 146.398	1.00 41.77	C	C
20	ATOM	4832	NE2	GLN	213			145.985	1.00 43.80 1.00 43.06	C	0
	ATOM	4833	C	GLN	213			145.792	1.00 43.00	C	N C
	ATOM	4834	0	GLN	213			146.792	1.00 32.23	C	0
	ATOM	4835	N	THR	214			147.930	1.00 32.37	c	И
30	ATOM	4836	CA	THR	214			149.103	1.00 30.20	C	C
- •	ATOM	4837	CB	THR	214			150.331	1.00 28.29	č	Č
	ATOM	4838	OG1		214			150.645	1.00 27.85	č	ŏ
	ATOM	4839	CG2	THR	214			150.047	1.00 28.08	Ċ	Ċ
	ATOM	4840	C	THR	214			149.509	1.00 27.47	Č	C
35	ATOM	4841	ō	THR	214			150.420	1.00 26.07	Ċ	ō
	ATOM	4842	N	GLN	215	11.842	-53.764	148.844	1.00 26.24	C	N
	ATOM	4843	CA	GLN	215	10.535	-53.196	149.175	1.00 27.14	С	С
	ATOM	4844	CB	GLN	215	9.433	-54.236	148.961	1.00 28.32	C	С
	ATOM	4845	CG	GLN	215	9.343	-54.776	147.533	1.00 32.89	С	C
40	ATOM	4846	CD	GLN	215	8.932	-53.716	146.532	1.00 34.61	C	C
	MOTA	4847	OE1	GLN	215	7.885	-53.085	146.676	1.00 36.92	C	0
	ATOM	4848	NE2	GLN	215			145.509	1.00 35.80	С	
	MOTA	4849	С	GLN	215			150.639	1.00 25.79	C	С
4-	MOTA	4850	0	GLN	215			151.318	1.00 25.44	C	0
45	MOTA	4851	N	ASN	216			151.103	1.00 24.70	С	N
	MOTA	4852	CA	ASN	216			152.467	1.00 24.04	С	С
	MOTA	4853	СВ	ASN	216			153.111	1.00 25.43	C	С
	ATOM	4854	CG	ASN	216			153.744	1.00 28.21	C	C
50	ATOM	4855		ASN	216			153.156	1.00 28.27	C	0
50	MOTA	4856	ND2		216			154.958	1.00 30.94	C	N
	ATOM	4857	C	ASN	216			L 152.406	1.00 21.89	C	C
	ATOM	4858		ASN	216			2 151.423	1.00 21.17	C	0
	MOTA	4859		PHE	217			153.460	1.00 20.68	C	N
55	ATOM	4860		PHE	217			153.538	1.00 20.49	C	C
33	ATOM	4861		PHE	217			3 154.171		C	C
	MOTA	4862		PHE	217			153.268	1.00 18.24	C	C
	MOTA	4863		PHE	217			9 153.209		C	C
	MOTA	4864	CD2	PHE	217	9.728	-45.92	1 152.472	1.00 19.04	C	С

-253-

	MOTA	4865	CE1	PHE	217	7.676	-47.783	152.366	1.00 20.17	С	C
	MOTA	4866		PHE	217		-45.706		1.00 18.75	C	C
	MOTA	4867	CZ	PHE	217		-46.636		1.00 18.41	С	C
_	MOTA	4868	С	PHE	217		-48.103		1.00 20.87	C	C
5	MOTA	4869	0	PHE	217		-48.577		1.00 19.76	C	0
	MOTA	4870	N	LEU	218		-47.592		1.00 21.69	C	N
	MOTA	4871	CA	LEU	218		-47.560		1.00 22.93	C	C
	MOTA	4872	СВ	LEU	218			153.910	1.00 24.83	С	С
40	MOTA	4873	CG	LEU	218			153.445	1.00 26.67	C	C
10	MOTA	4874	CD1		218			152.686	1.00 28.70	C	C
	MOTA	4875	CD2		218			152.547	1.00 27.72	C	С
	MOTA	4876	С	LEU	218			155.429	1.00 23.17	C	C
	MOTA	4877	0	LEU	218			154.760	1.00 22.44	C	0
4.5	MOTA	4878	N	CYS	219			156.732	1.00 23.14	C	N
15	MOTA	4879	CA	CYS	219			157.435	1.00 24.43	C	С
	MOTA	4880	CB	CYS	219			158.052	1.00 23.99	C	C
	MOTA	4881	SG	CYS	219			156.826	1.00 21.86	C	S
	MOTA	4882	С	CYS	219			158.503	1.00 24.72	C	C
	MOTA	4883	0	CYS	219			159.651	1.00 24.29	C	0
20	MOTA	4884	N	GLY	220			158.105	1.00 24.82	C	N
	MOTA	4885	CA	GLY	220			159.011	1.00 24.67	C	C
	MOTA	4886	C	GLY	220			159.323	1.00 23.88	C	C
	MOTA	4887	0	GLY	220			158.409	1.00 23.43	C	0
05	MOTA	4888	N	PRO	221			160.599	1.00 23.24	C	N
25	MOTA	4889	CD	PRO	221			161.801	1.00 23.12	C	C
	MOTA	4890	CA	PRO	221			160.913	1.00 22.65	C	С
	MOTA	4891	CB	PRO	221			162.272	1.00 22.04	С	С
	MOTA	4892	CG	PRO	221			162.926	1.00 21.62	C	С
20	MOTA	4893	C	PRO	221			160.964	1.00 22.50	C	C
30	MOTA	4894	0	PRO	221			161.265	1.00 22.01	C	0
	MOTA	4895	N	LEU	222			160.671	1.00 21.70	C	N
	ATOM	4896	CA	LEU	222			160.721	1.00 21.85	C	C
	MOTA	4897	СВ	LEU	222			161.316	1.00 21.57	C	C
25	MOTA	4898	CG	LEU	222			162.700	1.00 20.39	C	C
35	MOTA	4899		LEU	222			163.131	1.00 20.86	C	C
	MOTA	4900		LEU	222			163.712	1.00 20.79	C	C
	ATOM	4901	C	LEU	222			159.363	1.00 21.95	C	C
	ATOM	4902	0	LEU	222			158.316	1.00 22.14	C	0
40	ATOM	4903	N	ARG	223			159.402	1.00 21.42	C	N
40	ATOM	4904	CA	ARG	223			158.198 157.921	1.00 21.84	C	C
	ATOM	4905	CB	ARG	223			157.921	1.00 23.26		
	MOTA	4906	CG	ARG	223 223			156.482	1.00 27.14		
	ATOM	4907 4908	CD NE	ARG ARG	223			156.393	1.00 30.23 1.00 32.56	C	C
45	MOTA		CZ	ARG	223			156.860	1.00 32.38	C	C
73	ATOM ATOM	4909 4910		ARG.	223			150.860	1.00 33.77	C	
	ATOM	4911		ARG	223			156.728	1.00 31.71	C	N
	MOTA	4912	C	ARG	223			5 158.381	1.00 33.10	C	C N
	MOTA	4913	Ö	ARG	223			159.290	1.00 20.43	C	o
50	ATOM	4913	И	TYR	224			5 157.517	1.00 20.43	C	N
00	ATOM	4915	CA	TYR	224			157.599	1.00 17.42	c	C
	ATOM	4916	CB	TYR	224			3 157.555 3 157.555	1.00 13.00	c	C
			CG	TYR	224			158.674	1.00 15.19	c	Č
	ATOM ATOM	4917 4918		L TYR	224			158.488	1.00 13.19	C	C
55	ATOM	4919		L TYR	224			9 159.514	1.00 15.25	C	C
33	MOTA	4920		2 TYR	224			5 159.924		C	C
	MOTA	4920		2 TYR	224			5 160.965		C	C
		4921		TYR	224			0 160.746		C	C
	MOTA	4744	CZ	IIK	224	10.613	, -40.43	J 100.746	T.00 T#133	C	C

-254-

	ATOM	4923	ОН	TYR	224	11 011	-45.570	161 740	1.00 13.71	С	0
	ATOM	4924	C	TYR	224		-51.312		1.00 15.26	Č	c
	ATOM	4925	ŏ	TYR	224		-51.087		1.00 12.96	c	ŏ
	ATOM	4926	N	THR	225			156.693	1.00 12.30	C	N
5	ATOM	4927	CA	THR	225			155.647	1.00 15.88	C	Ċ
•	ATOM	4928	CB	THR	225		-54.639		1.00 15.32	c	Č
	MOTA	4929	OG1	THR	225		-55.067		1.00 15.32	C	ŏ
	MOTA	4930	CG2	THR	225		-54.799		1.00 15.24	C	č
	MOTA	4931	C	THR	225			155.592	1.00 13.24	C	C
10	ATOM	4932	0	THR	225			156.433	1.00 13.09	C	Ö
10	ATOM	4932	N	ILE	226			154.609	1.00 14.59	c	N
	ATOM	4934	CA	ILE	226			154.465	1.00 14.58	C	C
	ATOM	4935	CB	ILE	226		-54.358	153.113	1.00 15.11	c	c
	ATOM	4936		ILE	226		-55.877		1.00 13.11	C	C
15	ATOM	4937		ILE	226		-53.929		1.00 12.89	C	c
13	ATOM	4938	CD1	ILE	226		-54.325	151.320	1.00 14.79	C	C
	ATOM	4939	CDI	ILE	226		-54.347	155.678	1.00 15.04	C	C
	ATOM	4940	0	ILE	226		-53.970	156.046	1.00 13.04	C	0
	MOTA	4941	N	GLU	227		-55.296	156.323	1.00 14.65	C	N
20	ATOM	4942	CA	GLU	227		-55.955	157.506	1.00 15.12	C	C
20	MOTA	4942	CB	GLU	227			158.006	1.00 15.12	C	C
	MOTA	4944	CG	GLU	227		-58.390		1.00 13.21	C	C
	ATOM	4945	CD	GLU	227			155.792	1.00 17.13	C	c
	ATOM	4946	_	GLU	227			155.700	1.00 20.90	C	õ
25	ATOM	4947		GLU	227			154.804	1.00 20.30	C	ŏ
25	ATOM	4948	C	GLU	227			158.654	1.00 14.83	C	C
	ATOM	4949	0	GLU	227			159.487	1.00 14.83	C	o
	ATOM .	4950	N	ASP	228		-53.893		1.00 14.73	C	N
	ATOM	4951	CA	ASP	228			159.793	1.00 15.26	c	C
30	ATOM	4952	CB	ASP	228			159.807	1.00 13.20	C	C
30	MOTA	4953	CG	ASP	228			160.109	1.00 14.01	C	C
	ATOM	4954		ASP	228			161.069	1.00 15.48	c	õ
	ATOM	4955		ASP	228			159.391	1.00 15.15	C	ŏ
	MOTA	4956	C	ASP	228			159.636	1.00 15.16	C	c
35	ATOM	4957	o	ASP	228			160.609	1.00 15.10	C	Ö
00	ATOM	4958	N	GLY	229			158.400	1.00 15.16	C	N
	MOTA	4959	CA	GLY	229			158.151	1.00 14.56	c	c
	ATOM	4960	C	GLY	229			158.416	1.00 14.33	c	C
	ATOM	4961	Ö	GLY	229			158.987	1.00 12.80	č	ŏ
40	ATOM	4962	N	ALA	230	0.623		158.023	1.00 13.05	Č	N
	ATOM	4963	CA	ALA	230			158.223	1.00 13.45	c	C
	ATOM	4964	CB	ALA	230			157.452	1.00 12.06	c	Č
	ATOM	4965	c	ALA	230			159.701	1.00 13.54	Č	Ċ
	ATOM	4966	ŏ	ALA	230			160.131	1.00 12.94	C	ō
45	MOTA	4967	N	ARG	231			160.482	1.00 13.80	Č	N
	ATOM	4968	CA	ARG	231			161.903	1.00 14.40	Č	C
	ATOM	4969	СВ	ARG	231			162.536	1.00 15.07	C	Č
	ATOM	4970	CG	ARG	231			3 162.018	1.00 16.54	C	Č
	ATOM	4971	CD	ARG	231			162.238	1.00 16.33	C	C
50	ATOM	4972	NE	ARG	231			5 163.632	1.00 16.45	C	N
	ATOM	4973		ARG	231			164.250		Č	C
	ATOM	4974		L ARG	231			5 163.611	1.00 17.87	Č	N
	ATOM	4975		2 ARG	231			3 165.514		c	N
	ATOM	4976		ARG	231			5 162.710		Č	C
55	ATOM	4977		ARG	231			2 163.797			Ö
	MOTA	4978		VAL	232			8 162.207			
	ATOM	4979			232			1 162.949			
	ATOM	4980		VAL	232			2 162.862			
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-255-

	MOTA	4981	CG1		232		-50.538		1.00 15.46		C
	MOTA	4982	CG2		232		-49.852		1.00 13.24		C
	MOTA	4983		VAL	232		-51.562		1.00 15.62		C
_	MOTA	4984		VAL	232		-50.718		1.00 14.53		0
5	MOTA	4985		GLY	233		-52.367		1.00 16.24		N
	MOTA	4986		GLY	233			161.104	1.00 17.01		С
	MOTA	4987		GLY	233		-51.859		1.00 17.97		C
	ATOM	4988	0	GLY	233		-51.926		1.00 18.13		0
40	MOTA	4989	N	PHE	234		-51.411		1.00 17.03		N
10	MOTA	4990	CA	PHE	234		-51.016		1.00 17.34		C
	MOTA	4991	CB	PHE	234		-50.295		1.00 17.03	C	C
	MOTA	4992	CG	PHE	234		-48.908		1.00 18.50	С	С
	MOTA	4993	CD1		234		-48.605		1.00 17.96	C	С
. =	ATOM	4994	CD2		234		-47.899		1.00 17.72	C	C
15	ATOM	4995		PHE	234		-47.310		1.00 19.80	C	C
	ATOM	4996		PHE	234		-46.604		1.00 18.38	С	C
	ATOM	4997	CZ	PHE	234			158.393	1.00 20.51	C	С
	MOTA	4998	С	PHE	234			156.703	1.00 18.19	С	С
	MOTA	4999	0	PHE	234			156.909	1.00 17.65	C	0
20	MOTA	5000	N	GLN	235	-5.298	-52.046	155.767	1.00 18.33	C	N
	MOTA	5001	CA	GLN	235			154.888	1.00 19.22	C	С
	MOTA	5002	CB	GLN	235			154.184	1.00 19.75	C	С
	MOTA	5003	CG	GLN	235			155.144	1.00 21.43	C	С
	ATOM	5004	CD	GLN	235			154.432	1.00 22.69	C	C
25	MOTA	5005	OE1	GLN	235	-9.633	-51.402	153.608	1.00 22.47	C	0
	MOTA	5006	NE2	GLN	235	-10.521	-53.118	154.751	1.00 22.23	С	N
	MOTA	5007	C	GLN	235	-4.637	-53.398	153.864	1.00 19.00	C	С
	MOTA	5008	0	GLN	235	-3.959	-52.486	153.393	1.00 17.75	C	0
	MOTA	5009	N	VAL	236			153.515	1.00 19.65	C	N
30	MOTA	5010	CA	VAL	236			152.564	1.00 19.44	C	C
	MOTA	5011	СВ	VAL	236	-3.408	-56.565	152.354	1.00 19.19	C	С
	MOTA	5012	CG1	VAL	236	-2.335	-56.927	151.320	1.00 17.93	C	C
	ATOM	5013	CG2	VAL	236			153.681	1.00 18.12	С	C
	ATOM	5014	С	VAL	236			151.218	1.00 19.53	C	C
35	ATOM	5015	0	VAL	236			150.648	1.00 18.39	C	0
	MOTA	5016	N	GLU	237			150.708	1.00 19.52	C	N
	MOTA	5017	CA	GLU	237			149.418	1.00 20.17	C	С
	ATOM	5018	CB	GLU	237			149.088	1.00 22.85	C	C
	MOTA	5019	CG	GLU	237			147.717	1.00 27.72	С	C
40	MOTA	5020	CD	GLU	237			147.431	1.00 31.75	C	C
	MOTA	5021	OE1		237			148.270	1.00 33.80	С	0
	MOTA	5022		GLU	237			146.371	1.00 33.68	С	0
	MOTA	5023	С	GLU	237			149.454	1.00 18.07	С	C
	MOTA	5024	0	GLU	237			148.534	1.00 16.31	С	0
45	MOTA	5025		PHE	238			150.515	1.00 16.98	С	N
	MOTA	5026		PHE	238			150.693	1.00 17.27	C	C
	ATOM	5027		PHE	238			5 152.027	1.00 17.34	C	C
	MOTA	5028		PHE	238			7 152.397	1.00 17.96	С	C
	MOTA	5029		PHE	238			7 151.694	1.00 18.18	C	C
50	MOTA	5030		PHE	238			7 153.421	1.00 18.28	С	C
	MOTA	5031		PHE	238			152.006	1.00 17.80	С	C
	MOTA	5032		PHE	238			2 153.743	1.00 18.89	C	C
	ATOM	5033		PHE	238			1 153.032	1.00 18.33	C	C
	MOTA	5034		PHE	238			3 150.703		C	C
55	MOTA	5035		PHE	238			3 150.008		C	0
	ATOM	5036		LEU	239			1 151.505		C	N
	ATOM	5037		LEU	239			0 151.615			С
	ATOM	5038	CB	LEU	239	-0.502	2 -52.21	2 152.598	1.00 15.80	С	С

-256-

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	MOTA	5039	CG	LEU	239		-51.903		1.00 17.46	С	C
	ATOM	5040	CD1		239		-50.502		1.00 15.39	C	C
	ATOM	5041	CD2		239		-52.946		1.00 16.59	С	С
-	MOTA	5042	С	LEU	239		-51.335		1.00 17.56	C	C
5	ATOM	5043	0	LEU	239	0.800	-50.696		1.00 17.19	C	0
	ATOM	5044	N	GLU	240	-0.757	-52.257	149.468	1.00 18.40	С	N
	ATOM	5045	CA	GLU	240	-0.230	-52.585	148.145	1.00 20.85	C	С
	MOTA	5046	СВ	GLU	240		-53.752		1.00 23.02	C	C
	MOTA	5047	CG	GLU	240		-55.083		1.00 26.39	Č	Ċ
10	MOTA	5048	CD	GLU	240		-55.778		1.00 30.97	Č	Ċ
	ATOM	5049	OE1		240		-55.087		1.00 32.51	č	ŏ
•	ATOM	5050	OE2	GLU	240		-57.028		1.00 32.31	Ċ	ŏ
	ATOM	5051	C	GLU	240		-51.366		1.00 20.90	C	c
	ATOM	5052	Ö	GLU	240		-51.126			c	
15									1.00 20.74		0
13	MOTA	5053	N	LEU	241		-50.596		1.00 21.07	C	N
	MOTA	5054	CA	LEU	241			146.501	1.00 22.58	C	C
	ATOM	5055	CB	LEU	241			146.741	1.00 24.26	С	С
	ATOM	5056	CG	LEU	241			146.093	1.00 26.53	C	C
00	MOTA	5057		LEU	241			144.575	1.00 27.75	C	С
20	MOTA	5058		LEU	241	-4.295	-46.683	146.513	1.00 28.98	C	C
	ATOM	5059	C	LEU	241	-0.369	-48.416	146.865	1.00 22.18	C	C
	MOTA	5060	0	LEU	241	0.233	-47.790	145.997	1.00 22.71	C	0
	MOTA	5061	N	LEU	242			148.158	1.00 20.92	C	N
	ATOM	5062	CA	LEU	242	0.946	-47.400	148.628	1.00 20.02	C	С
25	ATOM	5063	СВ	LEU	242	0.860	-47.274	150.153	1.00 20.07	С	C
	ATOM	5064	CG	LEU	242	1.789	-46.252	150.806	1.00 21.59	C	С
	MOTA	5065	CD1	LEU	242			150.189	1.00 20.97	С	C
	ATOM	5066		LEU	242			152.299	1.00 19.92	C	C
	ATOM	5067	C	LEU	242			148.196	1.00 19.08	Č	Č
30	ATOM	5068	ō	LEU	242			147.680	1.00 18.08	č	ŏ
	ATOM	5069	N	PHE	243			148.396	1.00 18.57	Č	N
	ATOM	5070	CA	PHE	243			148.006	1.00 18.80	č	C
	ATOM	5071	CB	PHE	243			148.603	1.00 16.93	C	c
	ATOM	5072	CG	PHE	243			150.053	1.00 15.95	C	C
35	MOTA	5072	CD1		243			151.049		C	C
00		5074	CD2						1.00 15.49		
	ATOM				243			150.410	1.00 14.54	С	C
	ATOM	5075	CE1		243			152.384	1.00 15.83	C	C
	ATOM	5076	CE2		243			151.738	1.00 15.46	C	C
40	ATOM	5077	CZ	PHE	243			152.732	1.00 14.97	C	C
40	ATOM	5078	C	PHE	243			146.484	1.00 19.80	С	C
	MOTA	5079	0	PHE	243			146.010	1.00 18.39	C	0
	ATOM	5080	N	HIS	244			145.720	1.00 20.82	C	
	ATOM	5081	CA	HIS	244			144.258	1.00 22.43	C	С
45	MOTA	5082	CB	HIS	244			143.609	1.00 25.14	С	C
45	MOTA	5083	CG	HIS	244			142.112	1.00 29.07	C	С
	MOTA	5084		HIS	244			141.269	1.00 30.07	С	С
	ATOM	5085		HIS	244			. 141.312	1.00 29.94	C	N
	ATOM	5086	CE1	. HIS	244			140.042	1.00 30.15	C	C
	ATOM	5087	NE2	HIS	244	2.276	-50.787	139.989	1.00 30.65	С	N
50	MOTA	5088	С	HIS	244	3.549	-48.353	143.834	1.00 21.93	C	C
	ATOM	5089	0	HIS	244	4.334	-48.125	142.914	1.00 21.81	C	0
	ATOM	5090	N	PHE	245			144.510	1.00 20.16	C	N
	ATOM	5091	CA	PHE	245			5 144.240	1.00 19.29	Č	C
	ATOM	5092	СВ	PHE	245			7 145.195	1.00 19.02	Č	Ċ
55	ATOM	5093	CG	PHE	245			7 145.238		c	Č
	ATOM	5094		PHE	245			7 144.242		C	C
	ATOM	5095		PHE	245			3 146.263		C	C
		5096		PHE				L 144.264		C	C
	MOTA	2020	CEL	. PRE	245	4.948	-41.40	144.204	1.00 10.07	C	Ü

-257-

	MOTA	5097	CE2		245	4.142 -41.913 146.300 1.00 18.71 C C	
	MOTA	5098	CZ	PHE	245	3.764 -41.020 145.295 1.00 19.85 C C	
	MOTA	5099	C	PHE	245	4.675 -45.727 144.470 1.00 18.96 C C	
E	MOTA	5100	0	PHE	245	5.355 -45.156 143.621 1.00 17.49 C O	
5	MOTA	5101	N	HIS	246	5.175 -46.138 145.633 1.00 17.92 C N	
	ATOM	5102	CA	HIS	246	6.577 -45.917 145.948 1.00 18.17 C C	
	MOTA	5103	CB	HIS	246	6.872 -46.353 147.382 1.00 17.39 C C	
	MOTA	5104	CG	HIS	246	6.504 -45.318 148.402 1.00 16.79 C C	
40	MOTA	5105	CD2		246	5.474 -45.253 149.279 1.00 16.89 C C	
10	ATOM	5106	ND1		246	7.211 -44.145 148.555 1.00 14.73 C N	
	ATOM	5107	CE1		246	6.631 -43.400 149.480 1.00 16.89 C C	
	ATOM	5108	NE2		246	5.574 -44.050 149.936 1.00 16.76 C N	
	ATOM	5109	C	HIS	246	7.533 -46.576 144.962 1.00 17.97 C C	
4 E	ATOM	5110	0	HIS	246	8.511 -45.968 144.560 1.00 17.61 C O	
15	ATOM	5111	N	GLY	247	7.243 -47.803 144.552 1.00 18.68 C N	
	MOTA	5112	CA	GLY	247	8.106 -48.462 143.587 1.00 19.53 C C	
	ATOM	5113	C	GLY	247	8.106 -47.744 142.243 1.00 20.19 C C	
	MOTA	5114	0	GLY	247	9.160 -47.522 141.646 1.00 20.80 C O	
20	MOTA	5115	N	THR	248	6.921 -47.373 141.765 1.00 19.87 C N	
20	ATOM	5116	CA	THR	248	6.778 -46.677 140.491 1.00 19.32 C C	
	MOTA	5117	CB	THR	248	5.281 -46.434 140.160 1.00 19.66 C C	
	MOTA	5118	OG1		248	4.577 -47.682 140.176 1.00 19.35 C O	
	MOTA	5119	CG2		248	5.127 -45.814 138.783 1.00 18.52 C C	
25	ATOM	5120	C	THR	248	7.519 -45.335 140.491 1.00 19.29 C C	
23	MOTA	5121	0	THR	248	8.259 -45.029 139.554 1.00 18.25 C O	
	ATOM	5122	N	LEU	249	7.320 -44.530 141.531 1.00 18.21 C N	
	ATOM	5123	CA	LEU	249	7.999 -43.238 141.604 1.00 19.06 C C	
	ATOM	5124	CB	LEU	249	7.520 -42.446 142.826 1.00 18.37 C C	
30	MOTA	5125	CG	LEU	249	8.207 -41.096 143.067 1.00 19.31 C C	
30	ATOM	5126		LEU	249	7.956 ~40.168 141.886 1.00 17.37 C C	
	ATOM	5127		LEU	249	7.677 -40.468 144.356 1.00 19.95 C C	
	MOTA	5128	C	LEU	249	9.518 -43.428 141.694 ·1.00 19.08 C C 10.278 -42.760 140.998 1.00 18.35 C O	
	MOTA	5129 5130	O N	LEU ARG	249 250	9.949 -44.342 142.555 1.00 19.05 C N	
35	ATOM ATOM	5130	CA	ARG	250	11.370 -44.605 142.748 1.00 21.51 C C	
00	ATOM	5132	CB	ARG	250	11.560 -45.712 143.793 1.00 22.24 C C	
	ATOM	5133	CG	ARG	250	13.002 -45.878 144.286 1.00 25.15 C C	
	ATOM	5134	CD	ARG	250	13.451 -44.658 145.095 1.00 27.57 C C	
	ATOM	5135	NE	ARG	250	14.457 -45.005 146.097 1.00 29.42 C N	
40	ATOM	5136	CZ	ARG	250	15.772 -44.954 145.909 1.00 31.82 C C	
70	ATOM	5137	-	ARG	250	16.272 -44.559 144.747 1.00 33.24 C N	
	ATOM	5138		ARG	250	16.594 -45.318 146.884 1.00 32.37 C N	
	ATOM	5139	C	ARG	250	12.069 -45.016 141.448 1.00 22.35 C C	
	ATOM	5140	Ö	ARG	250	13.192 -44.592 141.182 1.00 21.30 C O	
45	ATOM	5141	N	LYS	251	11.396 -45.835 140.640 1.00 23.28 C N	
	ATOM	5142	CA	LYS	251	11.973 -46.311 139.385 1.00 24.95 C C	
	ATOM	5143	СВ	LYS	251	11.072 -47.375 138.750 1.00 25.59 C C	
	ATOM	5144	CG	LYS	251	11.096 -48.727 139.454 1.00 27.12 C C	
	ATOM	5145	CD	LYS	251	10.179 -49.729 138.759 1.00 29.13 C C	
50	ATOM	5146	CE	LYS	251	9.952 -50.967 139.620 1.00 30.83 C C	
•	ATOM	5147	NZ	LYS	251	8.907 -51.877 139.064 1.00 31.97 C N	
	ATOM	5148		LYS	251	12.262 -45.222 138.359 1.00 25.23 C C	
	ATOM	5149		LYS	251	13.053 -45.437 137.439 1.00 25.25 C O	
	ATOM	5150		LEU	252	11.631 -44.059 138.511 1.00 24.72 C N	
55	ATOM	5151		LEU	252	11.843 -42.960 137.577 1.00 25.19 C C	
	ATOM	5152		LEU	252	10.683 -41.966 137.668 1.00 24.25 C C	
	ATOM	5153		LEU	252	9.307 -42.516 137.278 1.00 25.10 C C	
	ATOM	5154		l LEU	252	8.227 -41.491 137.611 1.00 24.20 C C	
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-258-

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	MOTA	5155	CD2		252		-42.861		1.00 24.17	C	C
	MOTA	5156	C	LEU	252		-42.232		1.00 26.15	C	C
	MOTA	5157	0	LEU	252		-41.354		1.00 26.54	C	0
_	MOTA	5158	N	GLN	253		-42.591		1.00 27.14	C	N
5	ATOM	5159	CA	GLN	253		-41.979		1.00 28.03	C	C
	MOTA	5160	CB	GLN	253	16.236	-42.492	138.159	1.00 29.58	C	C
	MOTA	5161	CG	GLN	253	16.524	-43.989	138.273	1.00 31.02	С	C
	ATOM	5162	CD	GLN	253	17.517	-44.495	137.228	1.00 33.14	C	С
	ATOM	5163		GLN	253		-45.643		1.00 35.27	Ċ	Ō
10	ATOM	5164			253		-43.644		1.00 33.37	c	N
	ATOM	5165	С	GLN	253		-40.461		1.00 27.47	č	C
	ATOM	5166	Ö	GLN	253			138.308	1.00 27.66	c	Ö
	ATOM	5167	N	LEU	254			139.876			
		5168							1.00 27.11	C	N
15	ATOM		CA	LEU	254		-38.428		1.00 26.74	C	C
13	ATOM	5169	CB	LEU	254			140.623	1.00 25.22	С	C
	ATOM	5170	CG	LEU	254			140.051	1.00 24.23	C	C
	MOTA	5171		LEU	254			140.762	1.00 22.94	C	С
	MOTA	5172		LEU	254			138.557	1.00 22.58	C	C
	MOTA	5173	C	LEU	254			140.528	1.00 27.44	C	C
20	MOTA	5174	0	LEU	254	15.953	-38.288	141.395	1.00 26.90	C	0
	MOTA	5175	N	GLN	255	15.535	-36.519	140.075	1.00 28.34	С	N
	MOTA	5176	CA	GLN	255	16.601	-35.708	140.625	1.00 30.41	C	C
	ATOM	5177	CB	GLN	255			139.542	1.00 32.70	С	C
	ATOM	5178	CG	GLN	255			138.521	1.00 35.87	C	C
25	ATOM	5179	CD	GLN	255			137.255	1.00 37.99	C	Ċ
	ATOM	5180		GLN	255			137.303	1.00 39.69	Č	ō
	ATOM	5181		GLN	255			136.111	1.00 39.40	c	N
	ATOM	5182	C	GLN	255			141.726	1.00 30.12	c	C
	ATOM	5183	ō	GLN	255			141.732	1.00 30.12	c	ŏ
30	MOTA	5184	N	GLU	256			142.658	1.00 29.99	C	N
00	MOTA	5185	CA	GLU	256 256			142.056			
									1.00 30.45	C	C
	MOTA	5186	CB	GLU	256			144.646	1.00 32.12	C	C
	MOTA	5187	CG	GLU	256			145.946	1.00 35.72	C	C
25	MOTA	5188	CD	GLU	256			146.936	1.00 37.90	C	С
35	ATOM	5189	OE1		256			146.676	1.00 39.48	С	0
	MOTA	5190	OE2		256			147.973	1.00 39.28	C	0
	ATOM	5191	С	GLU	256			143.354	1.00 29.53	С	C
	MOTA	5192	0	GLU	256			143.946	1.00 28.88	C	0
	MOTA	5193	N	PRO	257			142.349	1.00 28.61	C	N
40	MOTA	5194	CD	PRO	257	16.778	-31.542	141.589	1.00 28.20	C	C
	MOTA	5195	CA	PRO	257	14.584	-30.603	141.976	1.00 27.69	С	C
	ATOM	5196	CB	PRO	257	15.295	-29.905	140.820	1.00 27.66	С	С
	ATOM	5197	CG	PRO	257	16.744	-30.090	141.169	1.00 28.71	C	C
	ATOM	5198	С	PRO	257	13.213	-31.141	141.570	1.00 26.87	C	C
45	MOTA	5199	0	PRO	257	12.187	-30.550	141.891	1.00 26.59	С	0
	ATOM	5200	N	GLU	258			140.858	1.00 25.85	C	N
	MOTA	5201	CA	GLU	258			140.418	1.00 24.88	C	C
	ATOM	5202	СВ	GLU	258			139.439	1.00 24.17	C	Ċ
	ATOM	5203	CG	GLU	258			138.205	1.00 25.10	Ċ	C
50	ATOM	5204	CD	GLU	258			137.360	1.00 26.23	Č	C
00	ATOM	5205		GLU	258			. 137.933	1.00 25.87	c	~
	ATOM	5205	OE		258 258			136.118	1.00 25.87	C	0
											0
	MOTA	5207	C	GLU	258			141.629	1.00 23.84	C	C
55	MOTA	5208	0	GLU	258			141.678	1.00 22.84	C	0
55	MOTA	5209	N	TYR	259			142.611	1.00 22.35	C	N
	MOTA	5210	CA	TYR	259			143.827	1.00 22.61	C	C
	ATOM	5211	CB	TYR	259			144.760	1.00 21.98	C	С
	MOTA	5212	CG	TYR	259	12.258	-36.588	3 144.617	1.00 21.14	С	С

-259-

	MOTA	5213	CD1		259			144.761	1.00 20.56		C
	MOTA	5214	CE1		259			144.691	1.00 18.62		C
	MOTA	5215		TYR	259			144.394	1.00 20.34		C
_	MOTA	5216	CE2	TYR	259			144.320	1.00 19.30		C
5	ATOM	5217	CZ	TYR	259			144.473	1.00 19.88	C	C
	MOTA	5218	OH	TYR	259			144.427	1.00 17.21	C	0
	MOTA	5219	C	TYR	259			144.582	1.00 22.27	С	C
	MOTA	5220	0	TYR	259			144.944	1.00 21.25	C	0
40	MOTA	5221	N	VAL	260			144.805	1.00 21.69	C	N
10	ATOM	5222	CA	VAL	260			145.551	1.00 21.85	C	C
	MOTA	5223	CB	VAL	260			146.028	1.00 21.84	С	C
	MOTA	5224		VAL	260			146.804	1.00 23.44	C	C
	ATOM	5225	CG2	VAL	260			144.853	1.00 21.89	C	C
45	MOTA	5226	C	VAL	260			144.779	1.00 21.44	С	C
15	MOTA	5227	0	VAL	260			145.376	1.00 19.91	C	0
	ATOM	5228	N	LEU	261			143.456	1.00 21.26	C	N
	MOTA	5229	CA	LEU	261			142.609	1.00 23.04	C	C
	MOTA	5230 5231	CB	LEU LEU	261 261			141.172 140.440	1.00 24.60 1.00 24.84	C	C C
20	ATOM		CG CD1		261 261			140.440	1.00 24.84	C	C
20	MOTA	5232 5233		LEU LEU	261 261			139.599	1.00 24.16	C	C
	MOTA MOTA	5234	CDZ	LEU	261			142.667	1.00 25.17	C	C
	ATOM	5235	o	LEU	261			142.611	1.00 22.74	C	Ö
	ATOM	5236	N	LEU	262			142.792	1.00 22.34	C	Ŋ
25	MOTA	5237	CA	LEU	262			142.732	1.00 23.07	c	C
20	MOTA	5238	CB	LEU	262			142.863	1.00 24.16	c	C
	MOTA	5239	CG	LEU	262			142.507	1.00 27.12	Č	Ċ
	ATOM	5240		LEU	262			141.135	1.00 26.19	č	Ċ
	ATOM	5241		LEU	262			142.514	1.00 26.28	Č	Ċ
30	ATOM	5242	C	LEU	262			144.205	1.00 22.78	Č	Ċ
	ATOM	5243	Ö	LEU	262			144.249	1.00 21.96	Č	ō
	ATOM	5244	N	ALA	263			145.279	1.00 21.56	C	N
	ATOM	5245	CA	ALA	263	5.960	-31.833	146.583	1.00 21.33	C	С
	ATOM	5246	СВ	ALA	263	7.063	-31.825	147.648	1.00 19.74	C	C
35	MOTA	5247	С	ALA	263	5.269	-30.469	146.531	1.00 20.96	C	C
	MOTA	5248	0	ALA	263	4.220	-30.278	147.148	1.00 20.00	C	0
	ATOM	5249	N	ALA	264	5.865	-29.527	145.798	1.00 20.08	C	N
	ATOM	5250	CA	ALA	264			145.663	1.00 21.05	C	C
	MOTA	5251	CB	ALA	264	6.243	-27.288	144.853	1.00 19.86	C	С
40	MOTA	5252	C	ALA	264			144.980	1.00 21.31	C	C
	MOTA	5253	0	ALA	264			145.394	1.00 21.71	C	0
	MOTA	5254		MET	265			143.928		C	
	MOTA	5255	CA	MET	265			143.210	1.00 21.67	С	С
45	MOTA	5256	CB	MET	265			141.980	1:00 22.87	C	С
45	MOTA	5257	CG	MET	265			140.838	1.00 25.80	С	C C S
	ATOM	5258	SD	MET	265			139.427	1.00 29.35	C	S
	MOTA	5259	CE	MET	265			3 138.513	1.00 26.54	C	C
	MOTA	5260	C	MET	265			5 144.128	1.00 20.81	C	С
50	MOTA	5261	0	MET	265			2 144.066	1.00 19.86	C	0
50	ATOM	5262		ALA	266			9 144.992	1.00 20.98	C	N
	MOTA	5263		ALA	266			145.922	1.00 21.57	C	C
	MOTA	5264		ALA	266			5 146.655 1 146 031	1.00 20.93	C	C
	ATOM	5265		ALA	266 266			l 146.931	1.00 21.45	C	C
55	MOTA	5266 5267		ALA	266 267			3 147.254 5 147.425	1.00 20.27 1.00 21.93	Ç	0
J	ATOM	5267		LEU LEU	267 267			147.425 4 148.391		C	C N
	MOTA MOTA	5268 5269		LEU	267 267			5 148.751		C	C
	MOTA	5269 5270		LEU	267			8 150.145		c	C
	AT ON	JZ 1 0			20,	2.333			2.00 23.70	~	_

-260-

	1.0014	C071	CD1		262	2 (10	05 011	150 100	1 00 00 05	_	_
	ATOM	5271		_	267			150.100	1.00 23.35	C	C
	ATOM	5272	CD2		267			150.605	1.00 23.37	C	C
	MOTA	5273	C	LEU	267			147.838	1.00 23.66	С	C
5	MOTA	5274	0	LEU	267			148.480	1.00 21.79	C	0
Э	ATOM	5275	N	PHE	268			146.645	1.00 25.33	С	N
	MOTA	5276	CA	PHE	268	-0.458	-25.881	146.031	1.00 27.92	C	С
	ATOM	5277	CB	PHE	268	0.358	-24.870	145.221	1.00 28.37	С	C
	MOTA	5278	CG	PHE	268	1.342	-24.097	146.048	1.00 28.12	C	С
	ATOM	5279	CD1	PHE	268	2.705	-24.256	145.856	1.00 27.58	С	С
10	ATOM	5280	CD2	PHE	268	0.900	-23.252	147.061	1.00 28.65	C	С
	ATOM	5281		PHE	268			146.664	1.00 28.19	С	C
	ATOM	5282		PHE	268			147.875	1.00 27.94	C	C
	ATOM	5283	CZ	PHE	268			147.678	1.00 28.60	Ċ	Č
	ATOM	5284	C	PHE	268			145.155	1.00 29.29	Č	Ċ
15	ATOM	5285	ŏ	PHE	268			143.935	1.00 28.87	c	Ö
	ATOM	5286	N	SER	269			145.800	1.00 28.87	C	N
	ATOM	5287	CA	SER	269			145.115			C
									1.00 33.69	С	
	MOTA	5288	CB	SER	269			145.616	1.00 33.87	C	C
20	MOTA	5289	OG	SER	269			145.148	1.00 34.33	C	0
20	ATOM	5290	С	SER	269			145.439	1.00 35.07	C	С
	MOTA	5291	0	SER	269			146.587	1.00 34.90	C	0
	MOTA	5292	N	PRO	270			144.423	1.00 36.60	C	N
	MOTA	5293	CD	PRO	270			143.018	1.00 36.73	С	C
	MOTA	5294	CA	PRO	270	-6.495	-25.254	144.528	1.00 37.91	С	C
25	MOTA	5295	CB	PRO	270	-6.556	-24.626	143.140	1.00 37.76	C	C
	ATOM	5296	CG	PRO	270	-6.115	-25.758	142.262	1.00 37.41	C	С
	ATOM	5297	С	PRO	270	-7.806	-25.925	144.911	1.00 39.15	С	С
	ATOM	5298	0	PRO	270			145.514	1.00 39.22	C	0
	ATOM	5299	N	ASP	271			144.565	1.00 40.15	C	N
30	ATOM	5300	CA	ASP	271			144.861	1.00 41.43	Č	C
	ATOM	5301	СВ	ASP	271			143.749	1.00 42.35	Č	Č
	ATOM	5302	CG	ASP	271			143.658	1.00 43.65	Č	Č
	ATOM	5302		ASP	271			143.728	1.00 43.56	c	ŏ
	ATOM	5304		ASP	271			143.499	1.00 44.16	C	ŏ
35	ATOM	5305	C	ASP	271			146.207	1.00 42.07	C	c
00											
	ATOM	5306	0	ASP	271			146.363	1.00 42.01	C	0
	ATOM	5307	N	ARG	272			147.178	1.00 42.23	C	N
	ATOM	5308	CA	ARG	272			148.516	1.00 42.88	C	C
40	ATOM	5309	СВ	ARG	272			149.139	1.00 42.11	C	С
40	MOTA	5310	CG	ARG	272			149.948	1.00 41.65	C	C
	MOTA	5311	CD	ARG	272			149.179	1.00 40.41	C	C
	ATOM	5312	NE	ARG	272			148.964	1.00 39.96	C	N
	MOTA	5313	CZ	ARG	272			148.563	1.00 38.64	С	C
45	MOTA	5314		L ARG	272			148.327	1.00 37.82	C	N
45	MOTA	5315	NH2	2 ARG	272			148.387	1.00 37.11	C	N
	ATOM	5316	С	ARG	272	-9.485	-28.073	149.385	1.00 44.03	C	C
	ATOM	5317	0	ARG	272	-9.942	-26.936	149.256	1.00 44.20	C	0
	ATOM	5318	N	PRO	273	-9.981	-28.933	150.284	1.00 44.99	C	N
	ATOM	5319	CD	PRO	273	-9.626	-30.349	150.507	1.00 45.02	С	C
50	MOTA	5320	CA	PRO	273	-11.093	-28.528	3 151.150	1.00 45.66	С	С
	MOTA	5321	СВ	PRO	273	-11.443	-29.819	151.894	1.00 45.44	C	С
	ATOM	5322		PRO	273			151.894	1.00 45.48	C	Ċ
	ATOM	5323	c	PRO	273			152.096	1.00 46.37	Č	c
	ATOM	5324		PRO	273			152.898	1.00 46.17	Č	ŏ
55	ATOM	5325		GLY	274			2 151.986	1.00 47.11	c	N
-0	ATOM	5326		GLY	274			152.839	1.00 47.72		C
				GLY	274			152.639	1.00 47.72		
	ATOM	5327								C	C
	MOTA	5328	0	GLY	274	-10.3/9	-22.90	3 152.830	1.00 48.57	C	0

-261-

	MOTA	5329	N	VAL	275	-10.113	-24.095	150.945	1.00 48.85	С	N
	ATOM	5330	CA	VAL	275		-23.016		1.00 49.89	С	C
	MOTA	5331	CB	VAL	275		-23.500		1.00 49.99	С	C
_	MOTA	5332	CG1		275		-24.549		1.00 50.05	С	C
5	MOTA	5333	CG2		275		-24.060		1.00 50.42	С	C
	ATOM	5334	C	VAL	275		-21.804		1.00 50.42	С	C
	MOTA	5335	0	VAL	275		-21.939		1.00 49.97	C	0
	ATOM	5336	N	THR	276		-20.620		1.00 51.16	C	N
40	MOTA	5337	CA	THR	276		-19.365		1.00 51.63	С	С
10	ATOM	5338	CB	THR	276		-18.333		1.00 51.76	C	С
	MOTA	5339		THR	276		-18.844		1.00 51.76	C	0
	ATOM	5340	CG2	THR	276		-17.027		1.00 52.34	C	C
	ATOM	5341	C	THR	276		-18.788		1.00 52.17	C	C
15	ATOM	5342	0	THR	276		-18.611		1.00 52.52	C	0
15	ATOM	5343	N	GLN	277		-18.498		1.00 52.57	C	N
	MOTA	5344	CA	GLN	277		-17.951		1.00 52.67	С	C
	MOTA	5345	CB	GLN	277		-17.195		1.00 53.56	C	C
	MOTA	5346	CG	GLN	277			147.596	1.00 55.26	C	C
20	MOTA	5347	CD	GLN	277			148.694	1.00 56.34	C	С
20	ATOM	5348		GLN	277			148.641	1.00 56.71	C	0
	ATOM	5349 5350	NE2 C		277			149.698 146.144	1.00 56.69	C	N C
	MOTA MOTA	5350	Ö	GLN GLN	277 277			145.144	1.00 52.40 1.00 51.95	C	0
	ATOM	5351	N		278			145.609	1.00 51.95	C	
25	MOTA	5352	CA	ARG ARG	278 278			143.609	1.00 52.21	C	И С
20	ATOM	5354	CB	ARG	278			144.226	1.00 52.47	C	C
	ATOM	5355	CG	ARG	278			143.568	1.00 56.61	C	C
	ATOM	5356	CD	ARG	278			143.074	1.00 58.62	C	C
	ATOM	5357	NE	ARG	278			142.770	1.00 60.54	C	N
30	ATOM	5358	CZ	ARG	278			142.245	1.00 61.18	Č	C
	ATOM	5359		ARG	278			141.949	1.00 61.12	č	N
	ATOM	5360		ARG	278			142.022	1.00 61.81	Č	N
	ATOM	5361	С	ARG	278			143.400	1.00 51.41	Ċ	C
	ATOM	5362	Ō	ARG	278			142.933	1.00 51.31	C	ō
35	ATOM	5363	N	ASP	279			142.861	1.00 50.43	C	N
	ATOM	5364	CA	ASP	279			141.668	1.00 48.92	C	С
	MOTA	5365	СВ	ASP	279	-8.122	-17.431	141.123	1.00 50.20	С	С
	MOTA	5366	CG	ASP	279	-9.497	-17.675	140.530	1.00 51.42	C	С
	MOTA	5367	OD1	ASP	279	-10.433	-17.982	141.296	1.00 52.30	C	0
40	MOTA	5368	OD2	ASP	279			139.294	1.00 52.68	C	0
	MOTA	5369	С	ASP	279	-6.000	-18.469	141.916	1.00 47.51	C	C
	MOTA	5370	0	ASP	279				1.00 47.56	C	_
	ATOM	5371	N	GLU	280			143.019	1.00 46.03	С	N
	MOTA	5372	CA	GLU	280			143.339	1.00 44.77	С	C
45	MOTA	5373	CB	GLU	280			144.614	1.00 46.49	C	C
	MOTA	5374	CG	GLU	280			145.185	1.00 48.88	С	С
	MOTA	5375	CD	GLU	280			146.331	1.00 50.21	С	C
	MOTA	5376		GLU	280			147.141	1.00 51.50	C	0
E 0	MOTA	5377		GLU	280			146.430	1.00 51.27	C	0
50	ATOM	5378	C	GLU	280			143.501	1.00 42.73	C	C
	ATOM	5379	0	GLU	280			142.994	1.00 42.02	C	0
	ATOM	5380	N	ILE	281			144.206	1.00 41.11	C	N
	ATOM	5381		ILE	281			3 144.414	1.00 40.07	C	C
55	ATOM	5382		ILE	281			2 145.439	1.00 38.98		C
33	ATOM	5383		2 ILE	281			5 145.480	1.00 37.84		C
	ATOM	5384 5305		LILE				1 146.820		C	
	ATOM	5385		LILE	281			1 147.882			
	MOTA	5386	С	ILE	281	-3.313	5 -21.83	5 143.081	1.00 40.18	С	С

-262-

	ATOM	5387	0	ILE	281	-2.318	-22.508	142.810	1.00 39.57	С	0
	MOTA	5388	N	ASP	282	-4.344	-21.692	142.252	1.00 40.74	С	N
	MOTA	5389	CA	ASP	282	-4.390	-22.319	140.934	1.00 41.64	C	C
_	ATOM	5390	CB	ASP	282		-21.949		1.00 44.29	C	C
5	MOTA	5391	CG	ASP	282	-6.024	-22.882	139.077	1.00 46.45	C	C
	ATOM	5392	OD1	ASP	282		-23.187		1.00 48.25	C	0
	MOTA	5393	QD2	ASP	282	-7.196	-23.305	138.977	1.00 48.22	С	0
	MOTA	5394	С	ASP	282	-3.208	-21.835	140.099	1.00 41.04	C	C
	MOTA	5395	0	ASP	282	-2.509	-22.629	139.470	1.00 40.33	С	0
10	MOTA	5396	N	GLN	283		-20.521		1.00 40.82	C	N
	MOTA	5397	CA	GLN	283	-1.899	-19.906	139.358	1.00 40.46	С	C
	ATOM	5398	CB	GLN	283	-1.966	-18.383	139.493	1.00 41.88	C	C
	ATOM	5399	CG	GLN	283	-0.695	-17.656	139.074	1.00 45.42	C	С
	MOTA	5400	CD	GLN	283	-0.388	-17.788	137.591	1.00 47.59	С	С
15	MOTA	5401	OE1	GLN	283	-0.244	-18.895	137.062	1.00 48.47	С	0
	ATOM	5402	NE2	GLN	283	-0.279	-16.652	136.913	1.00 49.11	C	N
	MOTA	5403	C	GLN	283	-0.557	-20.408	139.879	1.00 39.02	С	С
	MOTA	5404	0	GLN	283	0.381	-20.626	139.110	1.00 38.65	С	0
	MOTA	5405	N	LEU	284	-0.470	-20.574	141.194	1.00 37.60	С	N
20	MOTA	5406	CA	LEU	284	0.752	-21.060	141.824	1.00 36.30	С	С
	ATOM	5407	CB	LEU	284	0.595	-21.036	143.346	1.00 36.28	C	С
	ATOM	5408	CG	LEU	284	1.311	-19.955	144.172	1.00 36.05	С	С
	ATOM	5409	CD1	LEU	284	1.559	-18.694	143.366	1.00 35.74	C	С
	MOTA	5410	CD2	LEU	284	0.474	-19.665	145.404	1.00 34.66	C	С
25	MOTA	5411	С	LEU	284	1.068	-22.476	141.349	1.00 35.48	C	C
	ATOM	5412	0	LEU	284	2.217	-22.789	141.044	1.00 34.73	C	0
	MOTA	5413	N	GLN	285			141.272	1.00 35.23	С	N
	ATOM	5414	CA	GLN	285			140.828	1.00 35.83	C	C
	MOTA	5415	СВ	GLN	285			140.923	1.00 36.09	C	C
30	ATOM	5416	CG	GLN	285			140.807	1.00 37.57	C	C
	MOTA	5417	CD	GLN	285			141.050	1.00 39.14	Č	Ċ
	ATOM	5418	OE1	GLN	285			141.555	1.00 40.08	C	0
	ATOM	5419	NE2		285			140.681	1.00 39.83	С	N
	ATOM	5420	С	GLN	285			139.401	1.00 35.60	C	C
35	MOTA	5421	0	GLN	285			139.096	1.00 35.31	C	0
	ATOM	5422	N	GLU	286	0.235	-23.920	138.526	1.00 35.27	C	N
	MOTA	5423	CA	GLU	286			137.142	1.00 35.56	C	C
	ATOM	5424	СВ	GLU	286			136.338	1.00 37.53	C	C
	MOTA	5425	CG	GLU	286	-0.646	-23.468	134.997	1.00 41.47	C	C
40	MOTA	5426	CD	GLU	286			133.838	1.00 44.16	C	C
	ATOM	5427	OE1	GLU	286			133.674	1.00 45.97	С	0
	ATOM	5428	OE2	GLU	286			133.078	1.00 45.32	C	0
	ATOM	5429	С	GLU	286			137.110	1.00 34.24	С	С
	ATOM	5430	0	GLU	286			136.325	1.00 33.97	C	0
45	MOTA	5431	N	GLU	287			137.968	1.00 33.47	C	N
	ATOM	5432	CA	GLU	287			138.048	1.00 33.05	C	С
	ATOM	5433	CB	GLU	287			139.131	1.00 34.71	C	C
	ATOM	5434	CG	GLU	287			138.713	1.00 38.06	C	C
	MOTA	5435	CD	GLU	287			139.858	1.00 40.74	C	C
50	MOTA	5436		GLU	287			140.535	1.00 41.79	C	0
	ATOM	5437	OE2		287			140.079	1.00 41.29	Ċ	ō
	ATOM	5438	C	GLU	287			138.389	1.00 31.74	C	Č
	ATOM	5439	ō	GLU	287			2 137.805	1.00 31.68	Č	ō
	ATOM	5440		MET	288			3 139.347	1.00 30.39	Č	N
55	ATOM	5441	CA	MET	288			3 139.751	1.00 29.43	C	C
	ATOM	5442		MET	288			7 140.936	1.00 29.48	Č	C
	ATOM	5443		MET	288			142.175	1.00 30.45		Č
	MOTA	5444		MET	288			7 142.830			s
							_				_

-263-

	MOTA	5445		MET	288		-22.620		1.00 33.			C
	ATOM	5446		MET	288		-26.160		1.00 28.			C
	ATOM	5447		MET	288		-26.608		1.00 27.		-	0
_	MOTA	5448		ALA	289		-26.478		1.00 28.			N
5	MOTA	5449		ALA	289		-27.399		1.00 29.			C
	MOTA	5450		ALA	289		-27.492		1.00 28.			C
	MOTA	5451	-	ALA	289		-26.983		1.00 29.			C
	MOTA	5452		ALA	289		-27.786		1.00 29.			0
	MOTA	5453		LEU	290		-25.725		1.00 30.			N
10	MOTA	5454		LEU	290		-25.196		1.00 32.		C	С
	MOTA	5455		LEU	290		-23.723		1.00 33.		С	C
	MOTA	5456		LEU	290		-23.411		1.00 35.		С	С
	ATOM	5457	CD1		290		-24.447		1.00 35.		C,	C
	MOTA	5458	CD2		290		-22.005		1.00 36.		C	С
15	MOTA	5459	С	LEU	290			134.569	1.00 32.		C	С
	MOTA	5460	0	LEU	290			133.734	1.00 32.		C	0
	MOTA	5461	N	THR	291			135.800	1.00 32.		С	N
	ATOM	5462	CA	THR	291			136.234	1.00 33.		С	C
	MOTA	5463	CB	THR	291			137.683	1.00 33.		С	C
20	ATOM	5464	OG1	THR	291	8.554	-23.303	137.783	1.00 32.	. 87	С	0
	MOTA	5465	CG2	THR	291			138.092	1.00 32.	. 59	C	С
	MOTA	5466	С	THR	291			136.147	1.00 33		C	С
	MOTA	5467	0	THR	291			135.722	1.00 32	.77	C	0
	MOTA	5468	N	LEU	292	8.458		136.556	1.00 33	. 66	С	N
25	ATOM	5469	CA	LEU	292	8.781	-28.931	136.500	1.00 33	. 98	С	С
	MOTA	5470	CB	LEU	292			137.092	1.00 34		C	C
	MOTA	5471	CG	LEU	292	7.987	-31.152	137.659	1.00 34	.71	C	С
	MOTA	5472	CD1	LEU	292	6.719	-31.972	137.772	1.00 34	.26	С	С
	MOTA	5473	CD2	LEU	292			136.782	1.00 34		С	С
30	MOTA	5474	C	LEU	292	8.999	-29.339	135.042	1.00 34	.02	С	C
	MOTA	5475	0	LEU	292			134.717	1.00 33	.46	C	0
	ATOM	5476	N	GLN	293	8.076	-28.936	134.173	1.00 34	.86	С	N
	MOTA	5477	CA	GLN	293	8.160	-29.261	132.752	1.00 36	.35	C	C
	MOTA	5478	CB	GLN	293	6.971	-28.679	131.991	1.00 36	.93	C	С
35	MOTA	5479	CG	GLN	293	5.626	-29.178	132.436	1.00 38	.19	C	С
	MOTA	5480	CD	GLN	293			131.612	1.00 39		C	C
	MOTA	5481	OE1	GLN	293	4.394	-28.839	130.409	1.00 39		C	0
	ATOM	5482	NE2	GLN	293	3.663	-27.772	132.254	1.00 39		C	N
	MOTA	5483	C	GLN	293	9.427	-28.683	132.161	1.00 37		С	C
40	ATOM	5484	0	GLN	293	10.218	-29.389	131.540	1.00 36	.18	C	0
	MOTA	5485	N	SER	294			132.353	1.00 38		C	N
	ATOM	5486	CA	SER	294			. 131.856	1.00 39		C	C
	MOTA	5487	CB	SER	294			132.343	1.00 39		C	C
	MOTA	5488	OG	SER	294			131.897	1.00 42		C	0
45	MOTA	5489	C	SER	294			. 132.333	1.00 39		С	С
	MOTA	5490	0	SER	294			131.559	1.00 39		C	0
	MOTA	5491	N	TYR	295			133.607	1.00 39		C	N
	MOTA	5492	CA	TYR	295	13.227	-28.382	134.160	1.00 39		C	C
	MOTA	5493	CB	TYR	295			3 135.674	1.00 37		C	C
50	MOTA	5494		TYR	295			3 136.310	1.00 35		C	C
	MOTA	5495		TYR	295			3 136.236			С	С
	MOTA	5496		TYR	295			2 136.787			C	С
	MOTA	5497		TYR	295			7 136.955			C	C
	MOTA	5498		TYR	295			137.506			С	С
55	MOTA	5499		TYR	295			3 137.420			C	С
	MOTA	5500		TYR				9 137.968			C	0
	MOTA	5501	C	TYR	295			5 133.501			С	C
	ATOM	5502	0	TYR	295	14.582	2 -30.13	7 133.283	1.00 41	09	C	0

WO 2005/019239 PCT/US2004/023092

-264-

	1 mov4	5503	NT.	77.0	206	12 261	30 445	122 200	1 00 40 17	_	
	ATOM		N	ILE	296			133.200	1.00 42.17	C	N
	MOTA	5504	CA	ILE	296			132.554	1.00 43.74	C	C
	MOTA	5505	СВ	ILE	296			132.634	1.00 42.58	С	C
_	MOTA	5506		ILE	296			131.723	1.00 41.40	C	C
5	MOTA	5507		ILE	296			134.083	1.00 41.48	C	С
	MOTA	5508	CD1	ILE	296	9.588	-33.749	134.268	1.00 39.89	C	C
	ATOM	5509	С	ILE	296	12.887	-31.587	131.089	1.00 45.95	C	С
	ATOM	5510	0	ILE	296	13.719	-32.347	130.593	1.00 45.55	С	0
	ATOM	5511	N	LYS	297	12.311	-30.605	130.399	1.00 48.91	С	N
10	ATOM	5512	CA	LYS	297			129.008	1.00 52.23	č	C
	ATOM	5513	СВ	LYS	297			128.441	1.00 51.99	č	č
	ATOM	5514	CG	LYS	297			128.141	1.00 52.84	C	C
		5515			297			127.281	1.00 52.84		
	ATOM		CD	LYS						C	C
45	MOTA	5516	CE	LYS	297			126.904	1.00 54.12	С	C
15	MOTA	5517	NZ	LYS	297			128.051	1.00 54.87	С	N
	ATOM	5518	С	LYS	297			129.014	1.00 54.53	С	С
	ATOM	5519	0	LYS	297	14.944	-30.844	128.441	1.00 55.09	C	0
	MOTA	5520	N	GLY	298	14.584	-28.997	129.661	1.00 57.15	C	N
	MOTA	5521	CA	GLY	298	16.003	-28.724	129.748	1.00 60.22	С	С
20	ATOM	5522	С	GLY	298	16.523	-29.978	130.411	1.00 62.54	С	С
	ATOM	5523	ō	GLY	298			131.358	1.00 62.69	Ċ	ō
	ATOM	5524	N	GLN	299			129.922	1.00 65.17	Č	N
	MOTA	5525	CA	GLN	299			130.525	1.00 67.96	Č	c
			-								
25	ATOM	5526	CB	GLN	299			132.033	1.00 68.38	C	C
23	MOTA	5527	CG	GLN	299			132.776	1.00 69.15	C	C
	MOTA	5528	CD	GLN	299			134.270	1.00 69.43	C	C
	MOTA	5529	OE1		299			134.788	1.00 69.78	C	0
	MOTA	5530	NE2	GLN	299	19.798	-32.317	134.973	1.00 69.64	C	N
	ATOM	5531	C	GLN	299	17.101	-32.871	130.246	1.00 69.68	C	C
30	MOTA	5532	0	GLN	299	16.567	-33.497	131.167	1.00 69.64	C	0
	ATOM	5533	N	GLN	300	16.827	-33.082	128.961	1.00 71.61	C	N
	ATOM	5534	CA	GLN	300			128.497	1.00 73.35	С	C
	ATOM	5535	СВ	GLN	300			127.502	1.00 73.72	Č	C
	ATOM	5536	CG	GLN	300			126.322	1.00 74.58	Č	č
35	MOTA	5537	CD	GLN	300			125.683	1.00 74.94	Č	Č
00				GLN	300			125.518		C	0
	ATOM	5538							1.00 74.96		
	MOTA	5539	NE2		300			125.313	1.00 75.16	C	N
	MOTA	5540	C	GLN	300			127.817	1.00 74.46	C	С
	MOTA	5541	0	GLN	300			126.943	1.00 74.52	C	0
40	MOTA	5542	N	ARG	301		-35.433		1.00 75.88	С	N
	MOTA	5543	CA	ARG	301			127.663	1.00 77.07	С	C
	MOTA	5544	CB	ARG	301	20.141	-36.271	128.128	1.00 77.84	С	C
	ATOM	5545	CG	ARG	301	20.867	-35.182	2 127.347	1.00 78.90	С	С
	MOTA	5546	CD	ARG	301	22.091	-34.650	128.082	1.00 79.88	С	С
45	ATOM	5547	NE	ARG	301	21.753	-33.619	129.060	1.00 80.47		N
	ATOM	5548	CZ	ARG	301			2 128.754	1.00 80.79		C
	ATOM	5549		ARG	301			2 127.488	1.00 80.67		N
	ATOM	5550		ARG	301			5 129.723	1.00 81.13		
								9 127.991			N
50	MOTA	5551	C	ARG	301				1.00 77.29		C
50	MOTA	5552	0	ARG	301			7 127.516	1.00 77.30		0
	MOTA	5553		ARG	302			3 128.809	1.00 77.38		N
	MOTA	5554		ARG	302			8 129.179	1.00 77.29		С
	MOTA	5555		ARG	302			2 130.036	1.00 77.61		С
	ATOM	5556	CG	ARG	302			0 130.578	1.00 78.03		C
55	ATOM	5557	CD	ARG	302	17.240	-38.61	4 131.998	1.00 78.58		C
	MOTA	5558		ARG	302			4 132.042	1.00 79.11		
	ATOM	5559		ARG	302			0 131.754			
	ATOM	5560		l ARG	302			0 131.406	1.00 79.26		
		2300	4444		342	~				•	

-265-

	ATOM	5561	NH2	ARG	302	20.148	-36.384	131.810	1.00 79.38	С	N
	ATOM	5562	C	ARG	302		-40.723		1.00 76.92	Ċ	C
	ATOM	5563	0	ARG	302		-40.166		1.00 77.08	C	0
	ATOM	5564	N	PRO	303		-41.991		1.00 76.31	Ċ	N
5	ATOM	5565	CD	PRO	303		-43.054	128.938	1.00 76.37	Č	C
	ATOM	5566	CA	PRO	303		-42.587		1.00 75.50	Ċ	Ċ
	ATOM	5567	СВ	PRO	303		-44.051		1.00 75.85	Ċ	С
	ATOM	5568	CG	PRO	303		-44.303		1.00 76.19	C	С
	ATOM	5569	C	PRO	303			125.957	1.00 74.45	Ċ	C
10	ATOM	5570	Ō	PRO	303	-		124.740	1.00 74.66	C	0
	ATOM	5571	N	ARG	304		-41.321		1.00 72.88	Ċ	N
	ATOM	5572	CA	ARG	304			126.185	1.00 71.00	С	C
	ATOM	5573	CB	ARG	304		-41.580	125.396	1.00 71.95	C	С
	ATOM	5574	CG	ARG	304		-42.797		1.00 72.83	Č	C
15	ATOM	5575	CD	ARG	304		-42.760		1.00 73.75	Ċ	Ċ
	ATOM	5576	NE	ARG	304		-42.747		1.00 74.86	Č	N
	ATOM	5577	CZ	ARG	304		-41.650		1.00 75.42	Č	C
	ATOM	5578		ARG	304		-40.437		1.00 75.19	C	N
	ATOM	5579	NH2	ARG	304	10.238	-41.763	122.880	1.00 75.41	C	N
20	ATOM	5580	С	ARG	304			127.189	1.00 68.99	C	C
	MOTA	5581	0	ARG	304			127.391	1.00 69.10	C	0
	ATOM	5582	N	ASP	305			127.783	1.00 66.12	C	N
	ATOM	5583	CA	ASP	305			128.758	1.00 62.53	C	С
	ATOM	5584	CB	ASP	305			130.145	1.00 64.03	С	C
25	ATOM	5585	CG	ASP	305			130.972	1.00 65.08	C	С
	MOTA	5586	OD1	ASP	305	10.994	-41.568	131.169	1.00 65.82	C	0
	MOTA	5587	OD2		305	13.167	-41.689	131.418	1.00 65.99	C	0
	ATOM	5588	С	ASP	305	10.965	-38.666	128.422	1.00 59.48	C	C
	MOTA	5589	0	ASP	305	11.262	-37.638	129.017	1.00 59.18	С	0
30	MOTA	5590	N	ARG	306	10.064	-38.713	127.450	1.00 55.57	C	N
	ATOM	5591	CA	ARG	306	9.266	-37.556	127.069	1.00 51.44	C	С
	MOTA	5592	CB	ARG	306	9.127	-37.474	125.568	1.00 53.15	C	C
	ATOM	5593	CG	ARG	306	8.361	-38.617	125.009	1.00 55.42	C	C
	MOTA	5594	CD	ARG	306	7.691	-38.219	123.755	1.00 57.72	C	C
35	ATOM	5595	NE	ARG	306	8.629	-38.071	122.651	1.00 59.57	C	N
	MOTA	5596	CZ	ARG	306	8.600	-38.822	121.560	1.00 60.42	C	C
	MOTA	5597	NH1	ARG	306	7.690	-39.766	121.445	1.00 61.04	С	N
	MOTA	5598	NH2	ARG	306	9.463	-38.620	120.579	1.00 61.02	C	N
	MOTA	5599	C	ARG	306	7.883	-37.863	127.671	1.00 47.25	С	C
40	ATOM	5600	0	ARG	306	6.933	-37.092	127.544	1.00 45.71	C	0
	MOTA	5601	N	PHE	307	7.808	-39.018	128.327	1.00 42.87	C	N
	MOTA	5602	CA	PHE	307			129.004	1.00 38.61	C	C
	MOTA	5603	CB	PHE	307			128.787	1.00 38.35	С	C
	ATOM	5604	CG	PHE	307			127.363	1.00 38.97	C	C
45	MOTA	5605		PHE	307			126.876	1.00 38.81	С	C
	MOTA	5606		PHE	307			126.497	1.00 38.13	С	С
	MOTA	5607		PHE	307			125.544	1.00 38.93	C	
	MOTA	5608	CE2		307			9 125.165	1.00 38.71	C	С
	MOTA	5609	CZ	PHE	307			124.687	1.00 38.27	C	C
50	MOTA	5610	С	PHE	307			130.499	1.00 35.65	C	
	ATOM	5611	0	PHE	307			5 131.273	1.00 35.24	C	
	ATOM	5612		LEU	308			5 130.893	1.00 32.79	C	
	MOTA	5613		LEU	308			132.299	1.00 30.05	С	
EF	MOTA	5614		LEU	308			5 132.459		C	
55	MOTA	5615		LEU	308			5 133.749			
	ATOM	5616		ren	308			5 134.243			
	ATOM	5617		2 LEU	308			1 134.833			
	ATOM	5618	C	LEU	308	7.224	-37.46	5 132.981	1.00 28.52	С	C

-266-

		5610	_		200	
	MOTA	5619	0	LEU	308	6.660 -37.796 134.026 1.00 26.62 C O
	ATOM	5620	N	TYR	309	7.022 -36.285 132.404 1.00 26.74 C N
	MOTA	5621	CA	TYR	309	6.110 -35.317 132.998 1.00 26.38 C C
_	MOTA	5622	CB	TYR	309	6.055 -34.046 132.147 1.00 26.27 C C
5	MOTA	5623	CG	TYR	309	5.169 -32.974 132.737 1.00 26.31 C C
	ATOM	5624		TYR	309	5.476 -32.390 133.966 1.00 25.78 C C
	MOTA	5625	CE1	TYR	309	4.647 -31.424 134.531 1.00 26.17 C C
	ATOM	5626	CD2	TYR	309	4.008 -32.561 132.082 1.00 26.61 C C
	MOTA	5627	CE2	TYR	309	3.170 -31.593 132.639 1.00 26.55 C C
10	ATOM	5628	CZ	TYR	309	3.497 -31.033 133.862 1.00 26.04 C C
	MOTA	5629	ОН	TYR	309	2.676 -30.088 134.423 1.00 26.95 C O
	MOTA	5630	С	TYR	309	4.704 -35.901 133.145 1.00 25.65 C C
	MOTA	5631	0	TYR	309	4.092 -35.805 134.206 1.00 24.69 C O
	MOTA	5632	N	ALA	310	4.202 -36.507 132.073 1.00 25.00 C N
15	ATOM	5633	CA	ALA	310	2.878 -37.113 132.091 1.00 25.46 C C
	ATOM	5634	CB	ALA	310	2.562 -37.742 130.721 1.00 23.32 C C
	ATOM	5635	c	ALA	310	2.789 -38.167 133.203 1.00 25.38 C C
	ATOM	5636	ŏ	ALA	310	1.793 -38.226 133.919 1.00 24.96 C O
20	ATOM	5637	N	LYS	311	
20	MOTA	5638	CA	LYS	311	3.835 -40.019 134.386 1.00 25.29 C C
	MOTA	5639	CB	LYS	311	5.072 -40.909 134.264 1.00 27.18 C C
	MOTA	5640	CG	LYS	311	5.041 -41.883 133.108 1.00 29.62 C C
	MOTA	5641	CD	LYS	311	6.294 -42.744 133.111 1.00 32.10 C C
0-	MOTA	5642	CE	LYS	311	6.291 -43.739 131.963 1.00 33.43 C C
25	MOTA	5643	NZ	LYS	311	7.545 -44.543 131.967 1.00 36.49 C N
	ATOM	5644	С	LYS	311	3.817 -39.386 135.785 1.00 24.36 C C
	MOTA	5645	0	LYS	311	3.206 -39.927 136.709 1.00 23.40 C O
	MOTA	5646	N	LEU	312	4.491 -38.250 135.938 1.00 22.72 C N
	ATOM	5647	CA	LEU	312	4.525 -37.566 137.227 1.00 22.36 C C
30	ATOM	5648	CB	LEU	312	5.615 -36.487 137.243 1.00 20.77 C C
	MOTA	5649	CG	LEU	312	7.066 -36.994 137.252 1.00 20.74 C C
	ATOM	5650	CD1	LEU	312	8.025 -35.805 137.282 1.00 19.34 C C
	ATOM	5651		LEU	312	7.300 -37.895 138.474 1.00 20.28 C C
	ATOM	5652	C	LEU	312	3.160 -36.961 137.568 1.00 22.23 C C
35	ATOM	5653	ō	LEU	312	2.787 -36.889 138.739 1.00 22.33 C O
••	ATOM	5654	N	LEU	313	2.415 -36.517 136.562 1.00 21.95 C N
	ATOM	5655	CA	LEU	313	1.087 -35.978 136.835 1.00 22.37 C C
	ATOM	5656	CB	LEU	313	0.499 -35.292 135.597 1.00 21.79 C C
	ATOM	5657	CG	LEU	313	1.160 -33.976 135.184 1.00 22.17 C C
40				LEU.	313	0.375 -33.363 134.037 1.00 22.22 C C
70	MOTA	5658 5659		LEU	313	1.200 -33.010 136.371 1.00 21.19 C C
	ATOM					
	ATOM	5660	C	LEU	313	0.200 -37.146 137.266 1.00 22.14 C C
	MOTA	5661	0	LEU	313	-0.610 -37.019 138.180 1.00 22.77 C O
AE	ATOM	5662	N	GLY	314	0.368 -38.288 136.609 1.00 21.90 C N
45	MOTA	5663	CA	GLY	314	-0.409 -39.458 136.965 1.00 22.13 C C
	MOTA	5664	C	GLY	314	-0.117 -39.885 138.393 1.00 22.23 C C
	MOTA	5665	0	GLY	314	-1.022 -40.283 139.124 1.00 21.32 C O
	MOTA	5666	N	LEU	315	1.153 -39.809 138.790 1.00 22.49 C N
	ATOM	5667	CA	LEU	315	1.550 -40.183 140.140 1.00 22.84 C C
50	MOTA	5668	СВ	LEU	315	3.077 -40.249 140.250 1.00 23.35 C C
	MOTA	5669	CG	LEU	315	3.674 -41.496 139.587 1.00 23.08 C C
	ATOM	5670	CD:	L LEU	315	5.189 -41.400 139.500 1.00 22.58 C C
	ATOM	5671	CD:	LEU	315	3.254 -42.716 140.396 1.00 22.20 C C
	ATOM	5672	C	LEU	315	0.978 -39.208 141.158 1.00 23.01 C C
55	ATOM	5673	0	LEU	315	0.611 -39.610 142.262 1.00 23.00 C O
	ATOM	5674		LEU	316	0.904 -37.929 140.793 1.00 22.90 C N
	ATOM	5675		LEU	316	0.329 -36.931 141.686 1.00 23.06 C C
	ATOM	5676		LEU	316	0.493 -35.518 141.116 1.00 22.05 C C
		20.0	CD	THO.	210	J.155 55.516 111.110 1.00 20.00 0 C

-267-

	MOTA	5677		LEU	316	1.871 -	34.892	141.360	1.00 23.73	С	C
	MOTA	5678	CD1		316			140.669	1.00 23.24	C	C
	MOTA	5679	CD2		316			142.861	1.00 23.94	C	C
_	MOTA	5680	С	LEU	316	-1.148 -			1.00 23.27	C	C
5	MOTA	5681	0	LEU	316	-1.690 -	37.080	142.981	1.00 22.65	C	0
	MOTA	5682	N	ALA	317	-1.797 -	37.715	140.817	1.00 23.25	C	N
	MOTA	5683	CA	ALA	317	-3.206 -	38.089	140.888	1.00 24.23	C	C
	MOTA	5684	CB	ALA	317	-3.747 -	38.378	139.489	1.00 22.85	C	C
	MOTA	5685	С	ALA	317	-3.335 -	39.331	141.775	1.00 24.41	C	C
10	MOTA	5686	0	ALA	317	-4.238 -	39.424	142.606	1.00 24.43	C	0
	MOTA	5687	N	GLU	318	-2.421 -	40.279	141.603	1.00 24.78	C	N
	MOTA	5688	CA	GLU	318	-2.438 -			1.00 26.34	C	C
	MOTA	5689	CB	GLU	318	-1.353 -	42.469	141.918	1.00 28.61	C	С
	MOTA	5690	CG	GLU	318	-1.413 -	-43.829	142.596	1.00 33.39	C	C
15	MOTA	5691	CD	GLU	318	-0.543 -			1.00 36.18	C	C
	MOTA	5692	OE1	GLU	318	-0.627 -	-44.984	140.665	1.00 38.18	C	0
	MOTA	5693	OE2	GLU	318	0.215 -	-45.571	142.603	1.00 38.68	C	0
	ATOM	5694	С	GLU	318	-2.227 -	-41.194	143.877	1.00 24.85	C	C
	MOTA	5695	0	GLU	318	-2.849 -	-41.810	144.740	1.00 23.99	C	0
20	MOTA	5696	N	LEU	319	-1.347 -	-40.241	144.165	1.00 23.52	C	N
	MOTA	5697	CA	LEU	319	-1.066 -	-39.850	145.541	1.00 23.29	C	С
	ATOM	5698	CB	LEU	319	0.106 -	-38.866	145.564	1.00 22.68	C	C
	ATOM	5699	ÇG	LEU	319	0.728 -	-38.525	146.917	1.00 23.73	C	C
	ATOM	5700	CD1	LEU	319			147.707	1.00 21.67	C	C
25	MOTA	5701	CD2	LEU	319	2.011 -	-37.730	146.683	1.00 23.23	C	C
	ATOM	5702	C	LEU	319	-2.330 -	-39.226	146.144	1.00 22.92	C	C
	ATOM	5703	0	LEU	319	-2.593 ·	-39.340	147.340	1.00 20.62	C	0
	ATOM	5704	N	ARG	320	-3.114	-38.569	145.297	1.00 23.19	C	N
	MOTA	5705	CA	ARG	320	-4.364	-37.967	145.727	1.00 24.36	C	C
30	MOTA	5706	CB	ARG	320	-4.968	-37.168	144.577	1.00 26.94	C	C
	ATOM	5707	CG	ARG	320	-6.167	-36.349	144.952	1.00 30.73	C	C
	MOTA	5708	CD	ARG	320	-5.770	-34.977	145.472	1.00 33.34	C	C
	ATOM	5709	NE	ARG	320	-6.959	-34.240	145.887	1.00 35.45	C	N
	MOTA	5710	CZ	ARG	320	-7.089	-32.919	145.846	1.00 36.12	C	C
35	MOTA	5711	NH1	ARG	320	-6.096	-32.157	145.403	1.00 36.02	C	N
	MOTA	5712	NH2	ARG	320	-8.222	-32.363	146.254	1.00 36.33	C	N
	MOTA	5713	С	ARG	320	-5.316	-39.099	146.148	1.00 23.68	C	C
	MOTA	5714	0	ARG	320	-6.003	-38.996	147.162	1.00 22.64	C	0
	MOTA	5715	N	SER	321	-5.350	-40.177	145.366	1.00 22.83	C	N
40	ATOM	5716	CA	SER	321	-6.194	-41.336	145.675	1.00 22.71	C	C
	MOTA	5717	CB	SER	321			144.571	1.00 22.94	C	C
	MOTA	5718	OG	SER	321	-6.657	-41.916	143.365	1.00 26.35	С	
	MOTA	5719	С	SER	321	-5.757	-41.973	146.985	1.00 21.50	С	C
	MOTA	5720	0	SER	321	-6.585	-42.420	147.766	1.00 21.06	С	0
45	MOTA	5721	N	ILE	322	-4.448	-42.031	147.208	1.00 20.81	С	N
	MOTA	5722	CA	ILE	322			148.428	1.00 20.53	С	C
	ATOM	5723	CB	ILE	322	-2.357	-42.707	148.336	1.00 20.88	C	С
	MOTA	5724	CG2		322	-1.741	-42.841	L 149.730			C
	MOTA	5725	CG1	ILE	322	-1.980	-43.902	2 147.444			С
50	MOTA	5726	CD1	LILE	322			5 147.088			C
	MOTA	5727	C	ILE	322			1 149.629			C
	ATOM	5728	0	ILE	322			L 150.693			0
	MOTA	5729		ASN	323			7 149.442			N
	MOTA	5730		ASN	323			3 150.478			С
55	MOTA	5731		ASN	323			9 149.925			С
	MOTA	5732		ASN	323	-5.148	-36.998	3 150.922			C
	MOTA	5733		l asn	323	-6.252	-37.08	7 151.463			
	MOTA	5734	ND2	2 ASN	323	-4.323	-35.98	5 151.151	1.00 29.48	C	N

-268-

	MOTA	5735	С	ASN	323	-6.172	-39.813	150.869	1.00 22.69	С	С
	MOTA	5736	0	ASN	323	-6.497	-39.936	152.053	1.00 22.78	C	0
	MOTA	5737	N	GLU	324	-7.025	-39.959	149.859	1.00 22.11	С	N
_	MOTA	5738	CA	GLU	324	-8.427	-40.294	150.070	1.00 23.38	С	C
5	ATOM	5739	CB	GLU	324	-9.186	-40.263	148.740	1.00 24.94	С	С
	ATOM	5740	CG	GLU	324	-9.451	-38.866	148.200	1.00 28.85	C	C
	MOTA	5741	CD	GLU	324	-10.021			1.00 31.28	С	C
	MOTA	5742	OE1	GLU	324	-10.867	-39.760	146.498	1.00 34.04	C	0
	ATOM	5743	OE2	GLU	324	-9.629	-38.028	145.976	1.00 32.20	C	0
10	ATOM	5744	С	GLU	324	-8.591	-41.673	150.714	1.00 22.12	C	C
	MOTA	5745	0	GLU	324	-9.446	-41.856	151.575	1.00 21.79	C	0
	MOTA	5746	N	ALA	325	-7.781	-42.641	150.297	1.00 20.25	C	N
	MOTA	5747	CA	ALA	325	-7.880	-43.982	150.869	1.00 20.09	C	C
	MOTA	5748	CB	ALA	325	-6.978	-44.958	150.112	1.00 20.27	C	C
15	MOTA	5749	С	ALA	325	-7.527	-43.946	152.354	1.00 19.28	C	С
	MOTA	5750	0	ALA	325	-8.133	-44.654	153.155	1.00 20.38	C	0
	MOTA	5751	N	TYR	326	-6.554	-43.121	152.728	1.00 18.75	C	N
	ATOM	5752	CA	TYR	326	-6.189	-42.974	154.140	1.00 19.01	С	C
	MOTA	5753	CB	TYR	326	-5.147	-41.869	154.325	1.00 18.00	C	C
20	ATOM	5754	CG	TYR	326	-3.719	-42.355	154.417	1.00 18.20	C	C
	MOTA	5755	CD1	TYR	326	-3.279	-43.109	155.513	1.00 17.45	С	С
	MOTA	5756	CE1	TYR	326	-1.943	-43.507	155.625	1.00 15.87	C	С
	MOTA	5757	CD2	TYR	326	-2.793	-42.022	153.433	1.00 17.03	C	C
	MOTA	5758	CE2	TYR	326	-1.466	-42.411	153.536	1.00 16.49	C	C
25	MOTA	5759	CZ	TYR	326	-1.045	-43.148	154.633	1.00 16.11	C	C
	MOTA	5760	ОН	TYR	326	0.281	-43.497	154.719	1.00 14.54	C	0
	MOTA	5761	С	TYR	326	-7.437	-42.601	154.936	1.00 19.02	C	C
	ATOM	5762	0	TYR	326	-7.673	-43.127	156.029	1.00 16.95	C	0
	ATOM	5763	N	GLY	327	-8.223	-41.676	154.382	1.00 18.76	C	N
30	MOTA	5764	CA	GLY	327	-9.448	-41.253	155.036	1.00 20.32	C	C
	ATOM	5765	С	GLY	327			155.263	1.00 21.04	C	С
	MOTA	5766	0	GLY	327	-10.973	-42.576	156.329	1.00 20.76	C	0
	MOTA	5767	N	TYR	328	-10.516	-43.289	154.257	1.00 21.82	С	N
	ATOM	5768	CA	TYR	328	-11.366	-44.463	154.398	1.00 22.78	C	С
35	MOTA	5769	CB	TYR	328	-11.461	-45.200	153.055	1.00 24.82	C	С
	ATOM	5770	CG	TYR	328			. 153.120	1.00 27.89	C	C
	MOTA	5771	CD1	. TYR	328			153.544	1.00 28.22	C	С
	MOTA	5772		. TYR	328			153.680	1.00 29.71	C	С
4.0	ATOM	5773		TYR	328			152.823	1.00 29.15	C	C
40	MOTA	5774	CE2		328		-47.693		1.00 30.37	C	С
	MOTA	5775	CZ	TYR	328			153.391	1.00 29.77	C	C
	MOTA	5776		TYR	328			153.567	1.00 31.94	С	-
	ATOM	5777	С	TYR	328			155.495	1.00 22.29	C	C
4-	MOTA	5778	0	TYR	328			3 156.391	1.00 21.48	C	0
45	MOTA	5779	N	GLN	329			3 155.427	1.00 22.12	C	N
	ATOM	5780	CA	GLN	329			156.424	1.00 22.84	C	C
	MOTA	5781	CB	GLN	329			L 156.205	1.00 21.43	C	С
	MOTA	5782	CG	GLN	329			2 154.901	1.00 20.52	С	С
50	MOTA	5783		GLN	329			154.789	1.00 21.36	C	С
50	MOTA	5784			329			3 153.889	1.00 21.96	C	0
	MOTA	5785			329			3 155.712	1.00 17.88	C	N
	MOTA	5786		GLN	329			3 157.846		C	C
	MOTA	5787		GLN	329			4 158.719		C	0
	MOTA	5788		ILE	330			3 158.070			N
55	ATOM	5789		ILE	330			9 159.382			C
	MOTA	5790		ILE	330			1 159.395			C
	MOTA	5791			330			4 160.470			C
	MOTA	5792	CG:	1 ILE	330	-7.196	-42.56	2 159.670	1.00 28.06	С	С

-269-

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	ATOM	5793	CD1		330		-43.192		1.00 29.01	C	С
	MOTA	5794	С	ILE	330	-10.634			1.00 26.85	С	C
	MOTA	5795	0	ILE	330	-10.879			1.00 24.12	С	0
_	MOTA	5796	N	GLN	331	-11.594			1.00 28.57	C	N
5	MOTA	5797	CA	GLN	331	-12.987			1.00 31.36	С	C
	MOTA	5798	CB	GLN	331	-13.887	-43.474	158.389	1.00 34.12	C	C
	MOTA	5799	CG	GLN	331	-14.097	-44.139	157.027	1.00 40.12	C	C
	MOTA	5800	CD	GLN	331	-15.111	-45.281	157.055	1.00 43.64	C	С
	MOTA	5801	OE1	GLN	331	-14.886	-46.346	156.463	1.00 46.08	C	0
10	ATOM	5802	NE2	GLN	331	-16.234	-45.062	157.737	1.00 45.76	C	N
	ATOM	5803	C	GLN	331	-13.455	-45.700	159.493	1.00 30.71	C	С
	ATOM	5804	0	GLN	331		-45.995		1.00 30.97	С	0
	ATOM	5805	N	HIS	332			158.801	1.00 30.40	C	N
	ATOM	5806	CA	HIS	332		-48.017		1.00 29.57	C	С
15	ATOM	5807	CB	HIS	332				1.00 30.43	Č	Ċ
	ATOM	5808	CG	HIS	332			157.209	1.00 32.56	Č	Ċ
	ATOM	5809		HIS	332			156.881	1.00 33.11	Č	c
	ATOM	5810		HIS	332			157.314	1.00 33.92	č	N
	ATOM	5811		HIS	332			157.057	1.00 33.97	č	c
20	ATOM	5812		HIS	332			156.791	1.00 33.45	C	N
20	ATOM	5813	C	HIS	332			159.861	1.00 28.67	C	Ċ
	ATOM	5814	Ö	HIS	332			160.333	1.00 28.07	c	Ö
	ATOM	5815	N	ILE	333			160.247	1.00 27.55	c	N
	ATOM	5816	CA	ILE	333			161.237	1.00 27.33	C	C
25		5817	CB	ILE	333			160.623	1.00 26.34	C	C
20	ATOM ATOM	5818	CG2		333			161.662	1.00 26.21	C	c
	ATOM	5819	CG2		333			159.447	1.00 25.58	C	C
				ILE	333			158.209	1.00 23.38	C	c
	ATOM	5820	CDI		333			162.519	1.00 24.80	C	C
30	ATOM ATOM	5821 5822		ILE	333			162.515	1.00 26.30	C	Ö
30		5823	N	GLN	334			163.605	1.00 25.96	C	N
	ATOM	5823		GLN	334			164.929	1.00 25.50	C	C
	MOTA		CA					165.923	1.00 28.84	C	C
	ATOM	5825	CB	GLN	334			165.325	1.00 28.84	C	c
35	ATOM	5826	CG	GLN	334				1.00 32.45		C
33	ATOM	5827	CD	GLN	334			168.254	1.00 36.09	C	0
	ATOM	5828	OE1		334			169.198		C	
	ATOM	5829	NE2		334			167.969	1.00 37.02	C	N
	ATOM	5830	С	GLN	334			165.394	1.00 25.97	C	C
40	MOTA	5831	0	GLN	334			165.271	1.00 25.42	C	0
40	MOTA	5832	N	GLY	335			165.919	1.00 25.33	C	N
	ATOM	5833	CA	GLY	335			166.392	1.00 24.56	C	C
	ATOM	5834		GLY	335			165.465	1.00 24.72	C	_
	MOTA	5835	0	GLY	335			165.917	1.00 24.71	C	0
4-	ATOM	5836		LEU	336			1 164.166	1.00 24.12	C	N
45	MOTA	5837		LEU	336			163.194	1.00 24.24	C	C
	MOTA	5838	СВ	LEU	336			3 161.771	1.00 23.67	C	C
	MOTA	5839		LEU	336			3 161.229	1.00 25.15	C	С
	ATOM	5840		LEU	336			5 159.795		С	С
	MOTA	5841		FEA TEA	336			7 161.277	1.00 24.69	С	C
50	MOTA	5842		LEU	336			5 163.390		С	
	MOTA	5843		LEU				2 163.348		С	0
	MOTA	5844		SER	337			0 163.598		C	
	MOTA	5845		SER				1 163.771			
	MOTA	5846	СВ	SER		-8.012	2 -41.93	1 164.044	1.00 23.77		
55	MOTA	5847	OG	SER	337	-8.473	3 -42.37	5 165.303	1.00 27.27		
	ATOM	5848	C	SER	337	-5.673	L -42.04	4 164.889	1.00 22.01		C
	ATOM	5849		SER		-5.089	-40.96	7 164.824	1.00 22.40	С	
	ATOM	5850		ALA				2 165.907		С	

-270-

	ATOM	5851	CA	ALA	338	-4.649	-42.568	167.038	1.00 21.23	С	C
	ATOM	5852	CB	ALA	338	-4.786	-43.660	168.118	1.00 19.99	С	С
	ATOM	5853	C	ALA	338	-3.170	-42.372	166.665	1.00 20.93	С	С
	ATOM	5854	0	ALA	338		-41.788		1.00 20.73	С	0
5	ATOM	5855	N	MET	339	-2.763	-42.862	165.494	1.00 21.18	С	N
	MOTA	5856	CA	MET	339	-1.380	-42.709	165.037	1.00 21.93	C	C
	ATOM	5857	CB	MET	339	-0.995	-43.866	164.117	1.00 20.73	C	С
	MOTA	5858	CG	MET	339	-0.835	-45.183	164.865	1.00 19.60	C	C
_	ATOM	5859	SD	MET	339	-0.305	-46.523	163.803	1.00 19.45	C	S
10	ATOM	5860	CE	MET	339	-1.798	-46.789	162.824	1.00 19.70	С	С
	ATOM	5861	С	MET	339	-1.146	-41.369	164.335	1.00 22.95	С	С
	ATOM	5862	0	MET	339	-0.029	-41.034	163.945	1.00 21.85	С	0
	MOTA	5863	N	MET	340	-2.219	-40.614	164.167	1.00 24.72	C	N
	MOTA	5864	CA	MET	340	-2.154	-39.292	163.568	1.00 27.94	C	С
15	MOTA	5865	CB	MET	340	-2.843	-39.296	162.207	1.00 27.04	С	C
	MOTA	5866	CG	MET	340	-2.692	-38.005	161.453	1.00 26.07	С	C
	MOTA	5867	SD	MET	340	-0.965	-37.738	161.038	1.00 25.64	C	S
	ATOM	5868	CE	MET	340	-1.132	-36.639	159.656	1.00 24.53	С	С
	MOTA	5869	C	MET	340	-2.965	-38.472	164.558	1.00 31.10	С	С
20	ATOM	5870	0	MET	340	-3.995	-37.911	164.193	1.00 29.95	С	0
	MOTA	5871	N	PRO	341	-2.499	-38.393	165.825	1.00 34.82	С	N
	MOTA	5872	CD	PRO	341	-1.062	-38.551	166.110	1.00 34.96	С	C
	MOTA	5873	CA	PRO	341	-3.138	-37.674	166.934	1.00 38.26	С	С
	MOTA	5874	CB	PRO	341	-1.981	-37.433	167.904	1.00 37.12	C	С
25	MOTA	5875	CG	PRO	341	-0.800	-37.386	167.016	1.00 35.89	С	C
	MOTA	5876	C	PRO	341	-3.801	-36.398	166.490	1.00 41.84	C	С
	MOTA	5877	0	PRO	341	-4.568	-36.386	165.531	1.00 43.72	C	0
	MOTA	5878	N	LEU	342	-3.555	-35.309	167.196	1.00 44.96	C	N
	MOTA	5879	CA	LEU	342	-4.134	-34.079	166.723	1.00 46.88	C	C
30	MOTA	5880	CB	LEU	342	-3.876	-32.930	167.708	1.00 48.46	C	С
	MOTA	5881	CG	LEU	342	-4.775	-32.923	168.952	1.00 49.28	С	C
	MOTA	5882	CD1	LEU	342	-4.242	-33.902	169.995	1.00 50.51	С	C
	ATOM	5883	CD2	LEU	342	-4.833	-31.520	169.532	1.00 50.29	С	C
	MOTA	5884	C	LEU	342	-3.331	-33.917	165.437	1.00 47.75	C	C
35	MOTA	5885	0	LEU	342	-2.870	-34.907	164.857	1.00 46.19	C	0
	MOTA	5886	N	LEU	343	-3.141	-32.691	164.982	1.00 48.81	С	N
	MOTA	5887	CA	LEU	343	-2.374	-32.508	163.767	1.00 49.66	С	С
	ATOM	5888	CB	LEU	343	-1.024	-33.243	163.875	1.00 47.94	C	С
	ATOM	5889	CG	LEU	343	0.102	-32.825	164.841	1.00 46.64	C	C
40	MOTA	5890		LEU	343			2 164.275	1.00 46.63	С	С
	MOTA	5891		LEU	343			166.230	1.00 46.74	C	С
	MOTA	5892	С	LEU	343			162.607	1.00 51.07	С	
	MOTA	5893	0	LEU	343			2 162.192	1.00 50.79	C	0
	MOTA	5894		GLN	344			1 162.125	1.00 53.04	С	N
45	MOTA	5895	CA	GLN	344			160.988	1.00 55.20	С	C
	ATOM	5896		GLN	344			2 159.782	1.00 55.64	С	С
	MOTA	5897	CG	GLN	344			159.666	1.00 56.26	С	C
	MOTA	5898	CD	GLN	344			1 158.953	1.00 57.17	С	C
	MOTA	5899			344			5 158.912	1.00 57.87	С	0
50	MOTA	5900			344			158.384	1.00 57.99	C	N
	MOTA	5901		GLN	344			3 161.207	1.00 56.43	С	С
	MOTA	5902		GLN	344			1 160.349	1.00 56.91	C	0
	MOTA	5903		GLU	345			0 162.343	1.00 57.98		Ŋ
	MOTA	5904		GLU	345			5 162.680	1.00 58.92		С
55	MOTA	5905		GLU				6 162.696	1.00 59.25		C
	MOTA	5906		GLU	345			0 163.412			C
	MOTA	5907		GLU	345			B 162.449			С
	MOTA	5908	OE:	L GLU	345	-8.396	-31.49	1 162.807	1.00 61.74	С	0

	MOTA	5909	OE2		345			161.336	1.00 61.02	C	0
	MOTA	5910	C	GLU	345			161.719	1.00 59.19	С	C
	MOTA	5911	0	GLU	345		-36.638		1.00 59.25	С	0
_	ATOM	5912	OXT		345	-7.281	-37.761	161.931	1.00 59.81	C	0
5	TER	5913		GLU	345					C	_
	MOTA	5914	CB	PRO	103	-18.301			1.00 85.60	D	С
	MOTA	5915	CG	PRO	103	-19.706			1.00 85.87	D	C
	MOTA	5916	C	PRO	103			125.789	1.00 84.96	D	C
40	MOTA	5917	0	PRO	103			126.588	1.00 85.09	D	0
10	MOTA	5918	N	PRO	103			124.910	1.00 85.59	D	N
	MOTA	5919	CD	PRO	103			124.343	1.00 85.67	D	С
	MOTA	5920	CA	PRO	103			125.986	1.00 85.36	D	С
	MOTA	5921	N .	VAL	104			124.722	1.00 84.12	D	N
45	MOTA	5922	CA	VAL	104			124.383	1.00 83.16	D	С
15	MOTA	5923	CB	VAL	104			124.512	1.00 83.15	D	С
	MOTA	5924		VAL	104			124.170	1.00 83.06	D	С
	ATOM	5925	CG2	VAL	104			123.588	1.00 83.15	D	С
	MOTA	5926	C	VAL	104	-13.719	-91.938	125.235	1.00 82.38	D	С
	MOTA	5927	0	VAL	104			124.709	1.00 82.56	D	0
20	ATOM	5928	N	GLN	105	-13.680	-91.678	126.541	1.00 81.19	D	N
	MOTA	5929	CA	GLN	105			127.423	1.00 79.59	D	C
	MOTA	5930	CB	GLN	105			127.082	1.00 80.41	D	C
	MOTA	5931	CG	GLN	105			127.413	1.00 81.01	D	C
	MOTA	5932	CD	GLN	105	-10.121	-93.381	128.905	1.00 81.38	D	C
25	MOTA	5933	OE1	GLN	105	-9.699	-92.494	129.648	1.00 81.47	D	0
	MOTA	5934	NE2	GLN	105	-10.452	-94.591	129.348	1.00 81.27	D	N
	MOTA	5935	C	GLN	105	-13.029	-92.153	128.912	1.00 77.80	D	C
	MOTA	5936	0	GLN	105	-12.190	-91.579	129.607	1.00 77.77	D	0
	MOTA	5937	N	LEU	106	-14.196	-92.573	129.394	1.00 75.34	D	N
30	ATOM	5938	CA	LEU	106	-14.548	-92.421	130.806	1.00 72.86	D	C
	MOTA	5939	CB	LEU	106			131.007	1.00 72.85	D	C
	ATOM	5940	CG	LEU	106	-17.068	-91.595	130.507	1.00 72.73	D	С
	MOTA	5941		LEU	106	-17.971	-90.477	131.006	1.00 72.42	D	C
	MOTA	5942	CD2	LEU	106	-17.083	-91.663	128.995	1.00 72.91	D	C
35	MOTA	5943	C	LEU	106			131.322	1.00 70.93	D	C
	MOTA	5944	0	LEU	106			131.588	1.00 70.45	D	0
	MOTA	5945	N	SER	107			131.450	1.00 68.94	D	N
	MOTA	5946	CA	SER	107			131.910	1.00 67.00	D	C
4.0	MOTA	5947	CB	SER	107			132.172	1.00 66.72	D	С
40	MOTA	5948	OG	SER	107			2 133.146	1.00 65.92	D	0
	MOTA	5949	С	SER	107			133.160	1.00 65.96	D	C
	MOTA	5950	0	SER	107			133.806	1.00 65.94	D	0
	MOTA	5951	N	LYS	108			133.489	1.00 64.35	D	N
	MOTA	5952	CA	LYS	108			134.669	1.00 62.78	D	C
45	MOTA	5953	CB	LYS	108			3 134.547	1.00 63.38	D	C
	MOTA	5954	CG	LYS	108			5 133.341	1.00 64.14	D	C
	MOTA	5955	CD	LYS	108			7 133.350	1.00 65.05	D	C
	MOTA	5956	CE	LYS	108			3 132.112	1.00 65.31	D	С
	MOTA	5957	NZ	LYS	108			2 130.858	1.00 65.55	D	N
50	MOTA	5958	С	LYS	108			5 135.917	1.00 61.20	D	C
	MOTA	5959	0	LYS	108			137.025	1.00 60.95	D	0
	MOTA	5960	N	GLU	109			7 135.731	1.00 59.39	D	N
	MOTA	5961	CA	GLU	109			2 136.840	1.00 57.92	D	С
~~	MOTA	5962	CB	GLU	109			1 136.392			С
55	ATOM	5963	CG	GLU	109			7 135.870	1.00 60.46		С
	MOTA	5964		GLU				9 134.372			С
	MOTA	5965		1 GLU	109			133.936			
	MOTA	5966	OE:	2 GLU	109	-11.344	1-100.22	8 133.626	1.00 61.74	D	0

-272-

	MOTA	5967	C	GLU	109	-13.182			1.00 56.28	D	C
	ATOM	5968	0	GLU	109	-13.311	-96.156	138.571	1.00 56.26	D	0
	ATOM	5969	N	GLN	110	-12.872	-95.476	136.473	1.00 53.97	D	N
	ATOM	5970	CA	GLN	110	-12.669	-94.090	136.868	1.00 51.62	D	C
5	ATOM	5971	CB	GLN	110	-11.900	-93.336	135.775	1.00 51.23	D	С
	MOTA	5972	CG	GLN	110	-12.575	-93.289	134.422	1.00 50.22	D	С
	ATOM	5973	CD	GLN	110	-11.624	-92.904	133.295	1.00 49.90	D	С
	ATOM	5974	OE1		110	-12.062			1.00 49.66	D	0
	ATOM	5975	NE2	GLN	110			133.528	1.00 49.10	D	N
10	ATOM	5976	C	GLN	110			137.190	1.00 50.17	D	c
	ATOM	5977	ŏ	GLN	110			137.893	1.00 49.22	D	ŏ
	ATOM	5978	N	GLU	111			136.683	1.00 48.81	D	N
	ATOM	5979	CA	GLU	111			136.984	1.00 47.31	D	C
	ATOM	5980	CB	GLU	111			136.020	1.00 47.31	D	C
15	ATOM	5981	CG	GLU	111			136.020	1.00 49.14	D	C
13											C
	MOTA	5982	CD	GLU	111			134.914	1.00 53.11	D	
	ATOM	5983		GLU	111			134.793	1.00 53.51	D	0
	MOTA	5984		GLU	111			134.126	1.00 53.59	D	0
20	MOTA	5985	С	GLU	111			138.440	1.00 45.08	D	C
20	ATOM	5986	0	GLU	111			139.127	1.00 44.43	D	0
	MOTA	5987	N	GLU	112			138.896	1.00 42.54	D	N
	MOTA	5988	CA	GLU	112			140.263	1.00 40.31	D	C
	MOTA	5989	CB	GLU	112			140.331	1.00 40.53	D	C
0-	MOTA	5990	CG	GLU	112			141.744	1.00 41.61	D	C
25	ATOM	5991	CD	GLU	112			142.629	1.00 41.94	D	С
	MOTA	5992		GLU	112			143.831	1.00 42.13	D	0
	MOTA	5993	OE2	GLU	112	-18.219	-97.081	142.129	1.00 41.78	D	0
	MOTA	5994	C	GLU	112	-15.425	-94.644	141.199	1.00 38.58	D	C
	ATOM	5995	0	GLU	112	-15.752	-94.396	142.358	1.00 37.73	D	0
30	MOTA	5996	N	LEU	113	-14.245	-94.289	140.690	1.00 36.41	D	N
	ATOM	5997	CA	LEU	113	-13.262	-93.541	141.469	1.00 34.41	D	C
	ATOM	5998	CB	LEU	113	-11.978	-93.348	140.660	1.00 34.39	D	C
	MOTA	5999	CG	LEU	113	-10.991	-92.312	141.214	1.00 34.64	D	C
	ATOM	6000	CD1	LEU	113	-10.423	-92.785	142.556	1.00 33.12	D	C
35	MOTA	6001	CD2	LEU	113	-9.879	-92.084	140.200	1.00 34.83	D	C
	MOTA	6002	C	LEU	113	-13.837	-92.169	141.840	1.00 33.24	D	C
	ATOM	6003	0	LEU	113	-13.663	-91.692	2 142.961	1.00 32.72	D	0
	ATOM	6004	N	ILE	114	-14.503	-91.534	140.881	1.00 31.70	D	N
	ATOM	6005	CA	ILE	114	-15.114	-90.233	3 141.109	1.00 31.14	D	C
40	ATOM	6006	СВ	ILE	114	-15.682	-89.644	139.794	1.00 30.51	D	C
	ATOM	6007	CG2	ILE	114			140.087	1.00 28.60	D	С
	MOTA	6008		LILE	114	-14.528	-89.234	1 138.870	1.00 30.78	D	
	ATOM	6009		LILE	114			L 137.532	1.00 29.75	D	C
	ATOM	6010	С	ILE	114			7 142.140	1.00 31.12	D	С
45	ATOM	6011	O	ILE	114			1 143.015	1.00 30.80	D	0
	ATOM	6012	N	ARG	115			5 142.035	1.00 30.77	D	N
	ATOM	6013	CA	ARG	115			7 142.968	1.00 30.08	D	C
	ATOM	6014	СВ	ARG	115			2 142.640	1.00 31.12	D	Č
	ATOM	6015	CG	ARG	115			0 143.393	1.00 32.38	D	Č
50	MOTA	6016	CD	ARG	115			3 143.216	1.00 33.88	D	c
-	ATOM	6017	NE	ARG	115			6 143.907	1.00 34.78	D	N
	ATOM	6018	CZ	ARG	115			1 145.232	1.00 35.85	D	C
		6018		1 ARG	115			0 146.048		D	N
	MOTA	6020		2 ARG	115			3 145.048		D	
55	ATOM										N
33	ATOM	6021		ARG	115			6 144.393		D	
	MOTA	6022		ARG	115			2 145.301		D	0
	MOTA	6023		THR	116			1 144.559		D	
	MOTA	6024	CA	THR	116	-15.850	92.70	5 145.837	1.00 27.53	D	С

-273-

	MOTA	6025		THR	116	-14.748			1.00 28.08	D	C
	MOTA	6026	OG1	THR	116	-15.353			1.00 30.70	D	0
	MOTA	6027	CG2	THR	116	-13.978	-93.964	146.978	1.00 29.30	D	C
	MOTA	6028	С	THR	116	-15.233	-91.439	146.435	1.00 26.60	D	C
5	MOTA	6029	0	THR	116	-15.435	-91.134	147.616	1.00 25.28	D	0
	MOTA	6030	N	LEU	117	-14.467	-90.715	145.622	1.00 24.99	D	N
	MOTA	6031	CA	LEU	117	-13.831	-89.486	146.080	1.00 23.90	D	C
	MOTA	6032	CB	LEU	117	-12.951	-88.902	144.969	1.00 22.02	D	C
	ATOM	6033	CG	LEU	117	-11.621	-89.624	144.740	1.00 20.36	D	C
10	MOTA	6034	CD1	LEU	117	-10.988	-89.149	143.448	1.00 19.86	D	С
	MOTA	6035	CD2	LEU	117	-10.698	-89.379	145.920	1.00 19.89	D	С
	ATOM	6036	С	LEU	117	-14.882	-88.469	146.493	1.00 23.81	D	С
	ATOM	6037	0	LEU	117			147.533	1.00 23.44	D	0
	MOTA	6038	N	LEU	118			145.668	1.00 23.97	D	N
15	ATOM	6039	CA	LEU	118			145.908	1.00 24.68	D	C
	ATOM	6040	СВ	LEU	118			144.680	1.00 26.07	D	Ċ
	ATOM	6041	CG	LEU	118			144.665	1.00 27.99	D	Ċ
	ATOM	6042		LEU	118			144.878	1.00 28.05	D	Ċ
	ATOM	6043		LEU	118			143.329	1.00 29.41	D	Č
20	ATOM	6044	c	LEU	118			147.144	1.00 24.04	D	Ċ
	ATOM	6045	ŏ	LEU	118			147.936	1.00 23.27	D	ŏ
	ATOM	6046	N	GLY	119			147.295	1.00 23.56	D	N
	ATOM	6047	CA	GLY	119			148.451	1.00 22.61	D	c
	ATOM	6048	C	GLY	119			149.714	1.00 22.12	D	č
25	ATOM	6049	Ö	GLY	119			150.610	1.00 21.52	D	ŏ
	MOTA	6050	N	ALA	120			149.776	1.00 21.08	D	N
	ATOM	6051	CA	ALA	120			150.931	1.00 21.42	D	C
	ATOM	6052	CB	ALA	120			150.761	1.00 20.72	D	C
	ATOM	6053	C	ALA	120			151.131	1.00 20.72	D	c
30	ATOM	6054	o	ALA	120			152.251	1.00 21.07	D	o
30	ATOM	6055	N	HIS	121			150.037	1.00 21.20	D	N
		6056	CA	HIS	121			150.037	1.00 21.91	D	C
	ATOM ATOM	6057	CB	HIS	121			148.734	1.00 22.79	D	c
	ATOM	6058	CG	HIS	121			148.680	1.00 23.76	D	C
35											C
33	ATOM	6059		HIS	121			148.980	1.00 25.00	D	
	ATOM	6060		HIS	121			148.300	1.00 25.79	D	N C
	MOTA	6061		HIS	121			148.366 148.777	1.00 25.43	D	
	MOTA	6062		HIS	121				1.00 26.28	D	N
40	ATOM	6063	C	HIS	121			150.674	1.00 22.33	D	C
40	ATOM	6064	0	HIS	121			151.557	1.00 21.50	D	0
	MOTA	6065	N	THR	122			150.156	1.00 21.62	D	N
	ATOM	6066	CA	THR				150.597		D	
	ATOM	6067	CB	THR	122			2 149.772	1.00 23.18	D	C
45	MOTA	6068	OG1		122			148.387	1.00 25.50	D	0
40	ATOM	6069	CG2		122			150.212	1.00 22.28	D	C
	MOTA	6070	C	THR	122			152.077	1.00 22.45	D	C
	ATOM	6071	0	THR	122			152.796	1.00 21.90	D	0
	ATOM	6072	N	ARG	123			3 152.527	1.00 21.68		N
50	MOTA	6073	CA	ARG	123			2 153.922			C
50	MOTA	6074		ARG	123			3 154.149	1.00 22.11		C
	MOTA	6075		ARG	123			153.500			
	MOTA	6076		ARG	123			5 153.975			C
	MOTA	6077		ARG	123			153.438			
	MOTA	6078		ARG	123			4 152.207			-
55	MOTA	6079		l arg	123			1 151.356			
	MOTA	6080		2 ARG	123			0 151.828			
	MOTA	6081	C	ARG	123			2 154.914			_
	MOTA	6082	0	ARG	123	-19.091	-85.24	5 155.929	1.00 22.70	D	0

-274-

	3.000	6003	••		101		05 604	154 604	4 00 00 33	_	
	ATOM	6083	N	HIS	124	-17.318			1.00 22.37	D	N
	ATOM	6084	CA	HIS	124	-16.359			1.00 22.99	D	C
	MOTA	6085	CB	HIS	124	-15.223			1.00 23.32	D	C
5	MOTA	6086	CG	HIS	124		-87.397		1.00 25.33	D	С
3	ATOM	6087	CD2		124	-16.458			1.00 24.81	D	С
	MOTA	6088	ND1		124		-88.505		1.00 25.61	D	N
	MOTA	6089	_	HIS	124		-89.561		1.00 25.40	D	С
	MOTA	6090		HIS	124		-89.179		1.00 24.90	D	N
40	MOTA	6091	C	HIS	124		-83.643		1.00 22.18	D	С
10	MOTA	6092	0	HIS	124		-82.975		1.00 22.39	D	0
	MOTA	6093	N	MET	125			154.038	1.00 21.09	D	N
	MOTA	6094	CA	MET	125			153.790	1.00 21.77	D	С
	MOTA	6095	CB	MET	125			152.992	1.00 21.06	D	C
	MOTA	6096	CG	MET	125			153.689	1.00 21.90	D	С
15	MOTA	6097	SD	MET	125	-11.145	-83.007	152.872	1.00 24.77	D	S
	MOTA	6098	CE	MET	125	-11.623	-83.594	151.192	1.00 24.05	D	С
	MOTA	6099	С	MET	125	-15.898	-80.833	153.128	1.00 21.17	D	C
	MOTA	6100	0	MET	125	-15.870	-79.681	153.549	1.00 21.24	D	0
	MOTA	6101	N	GLY	126	-16.654	-81.220	152.104	1.00 21.62	D	N
20	MOTA	6102	CA	GLY	126	-17.499	-80.296	151.364	1.00 22.06	D	С
	MOTA	6103	C	GLY	126	-18.159	-79.155	152.113	1.00 23.28	D	C
	ATOM	6104	0	GLY	126	-18.209	-78.027	151.619	1.00 23.14	D	0
	ATOM	6105	N	THR	127	-18.694	-79.433	153.296	1.00 23.58	D	N
	ATOM	6106	CA	THR	127	-19.340	-78.387	154.071	1.00 24.53	D	С
25	ATOM	6107	CB	THR	127	-20.870	-78.636	154.170	1.00 25.29	D	C
	ATOM	6108	OG1	THR	127	-21.119	-80.020	154.456	1.00 25.66	D	0
	ATOM	6109	CG2	THR	127	-21.560	-78.260	152.856	1.00 25.86	D	C
	ATOM	6110	С	THR	127			155.473	1.00 24.35	D	C
	ATOM	6111	0	THR	127			156.387	1.00 24.95	D	0
30	ATOM	6112	N	MET	128			155.651	1.00 23.31	D	N
	ATOM	6113	CA	MET	128			156.969	1.00 22.39	D	C
	ATOM	6114	СВ	MET	128			156.981	1.00 21.54	D	Ċ
	ATOM	6115	CG	MET	128			156.440	1.00 19.76	D	C
	ATOM	6116	SD	MET	128			156.386	1.00 18.11	D	S
35	ATOM	6117	CE	MET	128			155.196	1.00 18.78	D	C
	ATOM	6118	C	MET	128			157.437	1.00 21.87	D	Č
	ATOM	6119	ŏ	MET	128			158.635	1.00 20.88	D	ō
	ATOM	6120	N	PHE	129			156.496	1.00 20.44	D	N
	ATOM	6121	CA	PHE	129			156.822	1.00 22.40	D	C
40	ATOM	6122	СВ	PHE	129			155.521	1.00 23.38	D	č
	ATOM	6123	CG	PHE	129			154.716	1.00 24.91	D	Č
	ATOM	6124	CD1		129			155.076	1.00 26.36	D	Č
	ATOM	6125		PHE	129			153.608	1.00 26.00	D	Č
	ATOM	6126	CE1		129			154.344	1.00 27.45	D	č
45	ATOM	6127	CE2		129			152.869	1.00 26.23	D	Č
	ATOM	6128	CZ	PHE	129			153.239	1.00 26.91	D	č
	ATOM	6129	C	PHE	129			157.682	1.00 22.06	D	č
	ATOM	6130	ŏ	PHE	129			158.394	1.00 20.89	D	ŏ
	ATOM	6131	N	GLU	130			157.625	1.00 23.03	D	N
50	ATOM	6132	CA	GLU	130			158.416	1.00 24.67	D	C
00	MOTA	6133	CB	GLU	130			157.978	1.00 26.82	D	Č
	ATOM	6134		GLU	130			156.573	1.00 20.82	D	C
		6135		GLU	130			L 156.467	1.00 32.46	D	C
	ATOM ATOM	6136		L GLU	130			7 157.480		D	0
55	ATOM	6137		2 GLU	130			5 155.362	1.00 34.27	D	0
55	ATOM	6138		GLU				155.362 1 159.916		ם	
	ATOM	6139								D	
				GLU				9 160.745		D	
	MOTA	6140	N	GLN	131	-10.90	-/3.36.	3 160.257	1.00 22.76	ע	N

-275-

	MOTA	6141	CA	GLN	131		-75.853		1.00 22.20	D	С
	MOTA	6142	CB	GLN	131	-17.967	-77.245	161.778	1.00 24.32	D	C
	MOTA	6143	CG	GLN	131	-18.846	-78.385	161.290	1.00 28.51	D	C
_	MOTA	6144	CD	GLN	131		-78.392		1.00 31.63	D	С
5	MOTA	6145	OE1		131		-78.373		1.00 34.51	D	0
	MOTA	6146	NE2		131		-78.420		1.00 32.89	D	N
	ATOM	6147	C	GLN	131		-74.843		1.00 20.71	D	C
	ATOM	6148	0	GLN	131		-74.829		1.00 19.33	D	0
40	MOTA	6149	N	PHE	132		-74.007		1.00 18.82	D	N
10	ATOM	6150	CA	PHE	132		-73.025		1.00 18.21	D	С
	ATOM	6151	СВ	PHE	132		-72.129		1.00 17.25	D	С
	ATOM	6152	CG	PHE	132		-72.825		1.00 16.76	D	С
	MOTA	6153		PHE	132		-74.133		1.00 15.85	D	C
45	ATOM	6154	CD2	PHE	132		-72.150		1.00 15.94	D	C
15	MOTA	6155	CE1	PHE	132		-74.762		1.00 16.23	D	С
	ATOM	6156	CE2	PHE	132		-72.772		1.00 16.64	D	C
	ATOM	6157	CZ	PHE	132		-74.078		1.00 15.57	D	C
	ATOM	6158	C	PHE	132		-72.159		1.00 17.13	D	C
20	ATOM	6159	0	PHE	132		-71.802		1.00 16.35	D	0
20	ATOM	6160	N	VAL	133		-71.832		1.00 16.80	D	N
	ATOM	6161	CA	VAL	133		-71.011		1.00 18.67	D	C
	ATOM	6162	CB	VAL	133			163.480	1.00 18.65	D	C
	ATOM	6163		VAL	133			163.626	1.00 18.17	D	C
25	ATOM	6164	CG2		133			164.272	1.00 21.43	D	C
25	ATOM	6165	C	VAL	133			165.327	1.00 18.01	D	C
	ATOM	6166	0	VAL	133			166.314	1.00 17.64	D	0
	ATOM	6167	N	GLN	134			165.383	1.00 17.24	D	N
	ATOM	6168	CA	GLN	134			166.631	1.00 18.01	D	C
30	ATOM	6169	CB	GLN	134			166.332	1.00 18.24	D	C
30	ATOM	6170	CG	GLN	134			165.643	1.00 20.23	D	C
	ATOM	6171	CD	GLN	134			166.579	1.00 20.77	D	С
	MOTA	6172	NE2	GLN	134			166.899	1.00 22.88	D	0
	MOTA	6173			134			167.032	1.00 20.71	D	N
35	MOTA MOTA	6174 6175	C	GLN	134			167.390	1.00 18.05	D	C
00	ATOM	6176	O N	GLN PHE	134 135			168.514 166.778	1.00 17.44	D	0
	ATOM	6177	CA	PHE	135			167.392	1.00 17.41	D D	N
	ATOM	6178	CB	PHE				166.412	1.00 17.91 1.00 16.42		C
	ATOM	6179	CG	PHE	135			166.091	1.00 15.42	D D	C
40	ATOM	6180		PHE	135			166.982	1.00 15.80	D	C
	ATOM	6181		PHE	135			164.942	1.00 15.41	D	C
	ATOM	6182		PHE	135			166.737	1.00 17.52	D	C
	ATOM	6183		PHE	135			164.678	1.00 17.32	D	c
	MOTA	6184	CZ	PHE	135			165.581	1.00 16.50	D	c
45	ATOM	6185	C	PHE	135			167.909	1.00 10.30	D	C
	ATOM	6186	ō	PHE	135			167.703	1.00 19.28	D	Ö
	ATOM	6187	N	ARG	136			168.590	1.00 19.27	D	N
	ATOM	6188	CA	ARG	136			169.198	1.00 20.81	D	C
	ATOM	6189	СВ	ARG	136			170.428	1.00 22.56	D	c
50	ATOM	6190	CG	ARG	136			171.538	1.00 26.27	D	C
	ATOM	6191	CD	ARG	136			172.275	1.00 30.26	D	Č
	ATOM	6192	NE	ARG	136			171.601	1.00 34.44	D	N
	ATOM	6193	CZ	ARG	136			171.612	1.00 36.40	D	C
	ATOM	6194		ARG	136			172.266	1.00 37.87	D	N
55	ATOM	6195		ARG	136			170.954	1.00 39.01	D	N
	ATOM	6196	С	ARG	136			168.261	1.00 20.52	D	C
	ATOM	6197	ō	ARG	136			168.529		D	
	ATOM	6198	N	PRO	137			167.151	1.00 20.21	D	
						,	55.25			_	

-276-

	MOTA	6199	CD	PRO	137	-16.587			1.00 20.40	D	С
	ATOM	6200	CA	PRO	137	-14.745			1.00 21.02	D	C
	ATOM	6201	CB	PRO	137	-15.646			1.00 20.72	D	C
_	MOTA	6202	CG	PRO	137	-16.973	-67.612	165.628	1.00 21.45	D	C
5	ATOM	6203	C	PRO	137	-14.806	-65.738	166.867	1.00 21.01	D	C
	MOTA	6204	0	PRO	137	-15.789	-65.373	167.509	1.00 20.39	D	0
	MOTA	6205	N	PRO	138	-13.735	-64.949	166.710	1.00 21.11	D	N
	MOTA	6206	CD	PRO	138	-12.375	-65.323	166.286	1.00 21.05	D	С
	ATOM	6207	CA	PRO	138	-13.764	-63.593	167.272	1.00 21.01	D	C
10	MOTA	6208	CB	PRO	138	-12.400	-63.036	166.890	1.00 21.60	D	С
	ATOM	6209	CG	PRO	138	-11.523	-64.269	166.967	1.00 22.95	D	С
	ATOM	6210	C	PRO	138	-14.914	-62.830	166.605	1.00 20.24	D	С
	ATOM	6211	0	PRO	138			165.490	1.00 17.44	D	0
	ATOM	6212	N	ALA	139	-15.419	-61.804	167.289	1.00 19.19	D	N
15	MOTA	6213	CA	ALA	139	-16.537	-60.991	166.804	1.00 17.76	D	С
	ATOM	6214	CB	ALA	139	-16.859	-59.892	167.827	1.00 17.06	D	С
	MOTA	6215	С	ALA	139	-16.346	-60.360	165.430	1.00 17.86	D	С
	MOTA	6216	0	ALA	139	-17.294	-60.281	164.645	1.00 17.93	D	0
	MOTA	6217	N	HIS	140	-15.133	-59.906	165.130	1.00 17.55	D	N
20	MOTA	6218	CA	HIS	140	-14.886	-59.266	163.842	1.00 16.71	D	С
	MOTA	6219	СВ	HIS	140	-13.507	-58.578	163.825	1.00 16.46	D	С
	ATOM	6220	CG	HIS	140	-12.363	-59.501	163.533	1.00 15.67	D	C
	ATOM	6221	CD2	HIS	140	-11.736	-59.798	162.371	1.00 14.99	D	С
	ATOM	6222	ND1	HIS	140	-11.745	-60.257	164.508	1.00 13.91	D	N
25	MOTA	6223	CE1	HIS	140	-10.786	-60.979	163.956	1.00 14.59	D	С
	MOTA	6224	NE2	HIS	140	-10.759	-60.719	162.661	1.00 15.09	D	N
	ATOM	6225	С	HIS	140	-15.013	-60.212	162.650	1.00 16.75	D	С
	MOTA	6226	0	HIS	140	-15.105	-59.764	161.513	1.00 15.99	D	0
	MOTA	6227	N	LEU	141	-15.033	-61.518	162.901	1.00 17.79	D	N
30	MOTA	6228	CA	LEU	141			161.814	1.00 18.75	D	C
	MOTA	6229	СВ	LEU	141	-14.682	-63.869	162.273	1.00 18.44	D	C
	MOTA	6230	CG	LEU	141	-13.186	-64.038	162.573	1.00 18.91	D	C
	ATOM	6231	CD1	LEU	141	-12.904	-65.504	162.883	1.00 17.51	D	C
	MOTA	6232	CD2	LEU	141	-12.345	-63.588	161.362	1.00 17.97	D	C
35	MOTA	6233	С	LEU	141	-16.588	-62.590	161.283	1.00 20.14	D	C
	MOTA	6234	0	LEU	141	-16.806	-63.055	160.167	1.00 19.48	D	0
	ATOM	6235	N	PHE	142	-17.565	-62.172	162.084	1.00 21.14	D	N
	ATOM	6236	CA	PHE	142	-18.950	-62.224	161.649	1.00 23.17	D	С
	MOTA	6237	CB	PHE	142	-19.908	-62.041	162.837	1.00 22.30	D	С
40	MOTA	6238	CG	PHE	142	-19.998	-63.249	163.726	1.00 22.33	D	С
	MOTA	6239	CD1	PHE	142	-19.018	-63.510	164.673	1.00 22.28	D	С
	MOTA	6240	CD2	PHE	142	-21.039	-64.158	163.578	1.00 22.17	D	C
	MOTA	6241	CE1	PHE	142			165.455	1.00 22.00	D	C
	MOTA	6242	CE2	PHE	142	-21.099	-65.301	164.353	1.00 20.89	D	С
45	MOTA	6243	CZ	PHE	142	-20.116	-65.550	165.293	1.00 21.02	D	C
	MOTA	6244	C	PHE	142	-19.229	-61.177	7 160.580	1.00 25.02	D	C
	MOTA	6245	0	PHE	142	-18.818	-60.018	3 160.692	1.00 24.19	D	0
	MOTA	6246	N	ILE	143	-19.924	-61.610	159.534	1.00 28.08	D	N
	MOTA	6247	CA	ILE	143			5 158.410		D	C
50	MOTA	6248	СВ	ILE	143	-21.243	-61.528	3 157.446	1.00 32.88	D	C
	MOTA	6249	CG2	ILE	143	-22.689	-61.262	2 157.814	1.00 33.01	D	C
	MOTA	6250		ILE	143			2 155.986		D	C
	ATOM	6251		ILE	143			1 155.606		D	С
	MOTA	6252	С	ILE	143			5 158.913		D	C
55	MOTA	6253		ILE	143			3 159.820		D	0
	MOTA	6254		HIS	144			3 158.334		D	N
	MOTA	6255	CA	HIS	144	-21.008	-57.00	3 158.680	1.00 34.98	D	C
	MOTA	6256	CB	HIS	144	-22.543	-56.99	3 158.683	1.00 37.72	D	

-277-

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	MOTA	6257	CG	HIS	144	-23.145			1.00 40.12	D	С
	MOTA	6258	CD2		144	-24.003			1.00 41.14	D	C
	MOTA	6259	ND1		144	-22.833			1.00 41.50	D	N
_	MOTA	6260	CE1		144	-23.470			1.00 41.78	D	C
5	ATOM	6261		HIS	144	-24.186			1.00 42.04	D	N
	ATOM	6262	C	HIS	144	-20.491	-56.424	159.990	1.00 34.54	D	С
	ATOM	6263	0	HIS	144	-20.892	-55.329	160.386	1.00 34.20	D	0
	ATOM	6264	N	HIS	145	-19.605	-57.147	160.666	1.00 33.54	D	N
	ATOM	6265	CA	HIS	145	-19.048	-56.650	161.916	1.00 32.95	D	С
10	ATOM	6266	СВ	HIS	145			162.865	1.00 32.61	D	C
	ATOM	6267	CG	HIS	145			164.287	1.00 32.37	D	Č
	ATOM	6268	CD2		145			165.386	1.00 32.00	D	Č
	ATOM	6269	ND1		145			164.704	1.00 32.66	D	N
	ATOM	6270		HIS	145			165.995	1.00 31.20	D	C
15	ATOM	6271		HIS	145			166.434	1.00 32.43	D	N
• •	ATOM	6272	C	HIS	145			161.605	1.00 32.43		C
	ATOM	6273	Ö	HIS	145					D	
	ATOM	6274	N					160.647	1.00 32.46	D	0
				GLN	146			162.417	1.00 32.73	D	N
20	ATOM	6275	CA	GLN	146			162.315	1.00 32.80	D	C
20	ATOM	6276	CB	GLN	146			163.466	1.00 36.08	D	С
	ATOM	6277	CG	GLN	146			163.823	1.00 40.75	D	C
	ATOM	6278	CD	GLN	146			164.913	1.00 42.71	D	С
	MOTA	6279	OE1		146			165.781	1.00 44.05	D	0
25	MOTA	6280	NE2		146			164.862	1.00 42.83	D	N
25	MOTA	6281	С	GLN	146			162.374	1.00 30.70	D	C
	MOTA	6282	0	GLN	146	-14.985	-55.716	163.093	1.00 29.52	D	0
	MOTA	6283	N	PRO	147	-14.067	-54.307	161.599	1.00 29.06	D	N
	ATOM	6284	CD	PRO	147	-14.144	-53.170	160.666	1.00 29.28	D	C
	MOTA	6285	CA	PRO	147	-12.738	-54.946	161.532	1.00 27.41	D	С
30	MOTA	6286	CB	PRO	147	-11.969	-54.050	160.559	1.00 27.81	D	C
	ATOM	6287	CG	PRO	147	-13.042	-53.488	159.682	1.00 28.67	D	С
	ATOM	6288	С	PRO	147	-12.040	-55.020	162.894	1.00 25.53	D	C
	ATOM	6289	0	PRO	147			163.831	1.00 26.05	D	0
	ATOM	6290	N	LEU	148	-11.008	-55.854	163.009	1.00 23.12	D	N
35	MOTA	6291	CA.	LEU	148			164.280	1.00 21.13	D	C
	ATOM	6292	СВ	LEU	148			164.231	1.00 20.59	D	C
	MOTA	6293	CG	LEU	148			165.532	1.00 20.63	D	Č
	MOTA	6294		LEU	148			166.595	1.00 18.94	D	Ċ
	ATOM	6295		LEU	148			165.270	1.00 20.92	D	Č
40	ATOM	6296	c	LEU	148			164.547	1.00 19.93	D	c
	ATOM	6297	ŏ	LEU	148			163.766	1.00 19.73	D	ŏ
	ATOM	6298	N	PRO	149			165.654	1.00 18.90	D	N
	ATOM	6299	CD	PRO	149			166.658	1.00 18.79	D	C
	ATOM	6300	CA	PRO	149			165.992	1.00 18.79	D	C
45	ATOM	6301	СВ	PRO	149			167.351	1.00 13.80	D	
	ATOM	6302	CG	PRO	149			167.331	1.00 17.91		C
	ATOM	6303								D	C
	ATOM		C	PRO	149			166.056	1.00 18.30	D	C
		6304	0	PRO	149			166.310	1.00 18.17	D	0
50	ATOM	6305	N	THR	150			165.837	1.00 19.06	D	N
50	ATOM	6306	CA	THR	150			165.870	1.00 18.45	D	C
	ATOM	6307	CB	THR	150			165.785	1.00 18.97	D	C
	MOTA	6308	OG1		150			164.469	1.00 16.80	D	
	ATOM	6309	CG2		150			166.110	1.00 16.34	D	
E E	ATOM	6310	C	THR	150			167.112	1.00 19.56	D	_
55	MOTA	6311	0	THR	150			167.003	1.00 20.79	D	_
	MOTA	6312	N	LEU	151			168.292	1.00 19.20	D	
	MOTA	6313	CA	LEU	151	-4.792	-52.451	169.518	1.00 19.49	D	С
	MOTA	6314	СВ	LEU	151			3 170.579	1.00 19.37	D	

-278-

	MOTA	6315		LEU	151		-50.116		1.00 19.71	D	C
	MOTA	6316	CD1		151		-49.078		1.00 19.45	D	C
	MOTA	6317	CD2		151		-50.542		1.00 19.57	D	С
_	ATOM	6318		LEU	151		-53.680		1.00 19.39	D	C
5	MOTA	6319		LEU	151		-54.136		1.00 18.10	D	0
	MOTA	6320		ALA	152		-54.220		1.00 18.60	D	N
	MOTA	6321		ALA	152		-55.396		1.00 18.53	D	C
	MOTA	6322	CB	ALA	152		-55.695		1.00 17.95	D	C
40	MOTA	6323	С	ALA	152			169.980	1.00 18.77	D	С
10	MOTA	6324	0	ALA	152		-56.815		1.00 18.21	D	0
	MOTA	6325	N	PRO	153			171.050	1.00 18.94	D	N
	MOTA	6326	CD	PRO	153			172.306	1.00 18.91	D	С
	MOTA	6327	CA	PRO	153			171.086	1.00 19.14	D	С
4 =	MOTA	6328	СВ	PRO	153			172.442	1.00 19.09	D	C
15	MOTA	6329	CG	PRO	153			173.283	1.00 20.56	D	С
	MOTA	6330	С	PRO	153			169.939	1.00 18.81	D	С
	MOTA	6331	0	PRO	153			169.589	1.00 17.99	D	0
	MOTA	6332	N	VAL	154			169.350	1.00 18.43	D	N
	MOTA	6333	CA	VAL	154			168.269	1.00 18.36	D	С
20	MOTA	6334	CB	VAL	154			167.166	1.00 18.03	D	C
	MOTA	6335		VAL	154			166.551	1.00 19.77	D	C
	MOTA	6336		VAL	154			167.747	1.00 17.94	D	С
	MOTA	6337	C	VAL	154			168.787	1.00 17.46	D	C
	ATOM	6338	0	VAL	154			168.047	1.00 16.70	D	0
25	MOTA	6339	N	LEU	155			170.053	1.00 17.73	D	N
	MOTA	6340	CA	LEU	155			170.637	1.00 18.30	D	C
	MOTA	6341	CB	LEU	155			172.156	1.00 18.87	D	С
	MOTA	6342	CG	LEU	155			172.949	1.00 18.81	D	С
00	MOTA	6343		LEU	155			172.393	1.00 18.11	D	С
30	MOTA	6344	-	LEU	155			174.426	1.00 19.81	D	С
	MOTA	6345	С	LEU	155			170.305	1.00 18.45	D	С
	MOTA	6346	0	LEU	155			169.897	1.00 19.26	D	0
	MOTA	6347	N	PRO	156			170.480	1.00 18.25	D	N
0.5	MOTA	6348	CD	PRO	156			171.115	1.00 17.28	D	C
35	MOTA	6349	CA	PRO	156			170.153	1.00 17.77	D	C
	MOTA	6350	CB	PRO	156			170.409	1.00 17.59	D	С
	ATOM	6351	CG	PRO	156			171.560	1.00 17.51	D	С
	ATOM	6352	C	PRO	156			168.714	1.00 17.24	D	C
40	MOTA	6353	0	PRO	156			168.458	1.00 16.32	D	0
40	MOTA	6354	N	LEU	157			167.780	1.00 16.35	D	N
	MOTA	6355	CA	LEU	157			166.374	1.00 15.67	D	С
	MOTA	6356		LEU	157			165.510		D	С
	ATOM	6357	CG	LEU	157			164.007	1.00 14.81	D	C
AE	ATOM	6358		LEU	157			163.411	1.00 13.61	D	C
45	MOTA	6359		LEU	157			163.337	1.00 14.21	D	C
	ATOM	6360	С	LEU	157			166.151	1.00 15.16	D	C
	ATOM	6361	0	LEU	157			165.405	1.00 14.60	D	0
	MOTA	6362		VAL	158			166.788	1.00 14.93	D	N
50	ATOM	6363		VAL	158			166.677	1.00 16.52	D	C
50	MOTA	6364		VAL	158			167.478	1.00 17.32	D	C
	MOTA	6365		. VAL	158			5 167.538	1.00 16.08	D	C
	ATOM	6366		VAL	158			166.825	1.00 15.99	D	C
	ATOM	6367		VAL	158			2 167.213	1.00 16.29	D	C
66	ATOM	6368		VAL	158			5 166.604			-
55	ATOM	6369		THR	159			3 168.350			Ŋ
	ATOM	6370		THR	159			9 168.959			_
	ATOM	6371		THR	159			2 170.352			
	MOTA	6372	OG1	LTHR	159	-6.190	-68.59	2 171.109	1.00 16.57	D	0

WO 2005/019239 PCT/US2004/023092

-279-

	ATOM	6373	CG2	THR	159	-7.501	-70.626	171.094	1.00 17.20	D	С
	ATOM	6374	C	THR	159	-7.680	-70.194	168.063	1.00 17.34	D	C
	MOTA	6375	0	THR	159	-7.794	-71.409	167.908	1.00 17.77	D	0
	ATOM	6376	N	HIS	160	-8.486	-69.315	167.478	1.00 16.89	D	N
5	ATOM	6377	CA	HIS	160	-9.541	-69.738	166.567	1.00 16.98	D	C
	ATOM	6378	CB	HIS	160	-10.363	-68.539	166.103	1.00 16.02	D	C
	MOTA	6379	CG	HIS	160	-11.374	-68.886	165.058	1.00 16.63	D	C
	MOTA	6380	CD2	HIS	160	-11.450	-68.560	163.746	1.00 16.70	D	С
	ATOM	6381	ND1	HIS	160	-12.451	-69.709	165.312	1.00 15.58	D	N
10	ATOM	6382	CE1	HIS	160	-13.146	-69.873	164.200	1.00 16.17	D	C
	MOTA	6383	NE2	HIS	160	-12.560	-69.187	163.235	1.00 15.22	D	N
	ATOM	6384	С	HIS	160	-8.933	-70.440	165.338	1.00 16.47	D	C
	ATOM	6385	0	HIS	160	-9.446	-71.459	164.881	1.00 15.93	D	0
	MOTA	6386	N	PHE	161	-7.855	-69.876	164.795	1.00 16.05	D	N
15	MOTA	6387	CA	PHE	161	-7.186	-70.473	163.645	1.00 16.40	D	С
	MOTA	6388	CB	PHE	161	-6.057	-69.564	163.125	1.00 15.95	D	С
	ATOM	6389	CG	PHE	161	-6.516	-68.474	162.172	1.00 15.49	D	C
	ATOM	6390		PHE	161	-7.819	-68.444	161.679	1.00 15.45	D	С
	MOTA	6391	CD2	PHE	161			161.739	1.00 15.30	D	С
20	ATOM	6392	CE1	PHE	161	-8.228	-67.458	160.763	1.00 14.86	D	С
	MOTA	6393	CE2	PHE	161			160.826	1.00 15.33	D	C
	ATOM	6394	CZ	PHE	161	-7.323	-66.487	160.338	1.00 14.34	D	С
	MOTA	6395	C	PHE	161			164.066	1.00 16.58	D	С
	MOTA	6396	0	PHE	161			163.377	1.00 16.53	D	0
25	ATOM	6397	N	ALA	162			165.199	1.00 16.50	D	N
	ATOM	6398	CA	ALA	162			165.687	1.00 16.70	D	C
	ATOM	6399	СВ	ALA	162			167.075	1.00 15.50	D	С
	ATOM	6400	C	ALA	162			165.750	1.00 16.99	D	C
	ATOM	6401	Ō	ALA	162			165.263	1.00 16.57	D	0
30	ATOM	6402	N	ASP	163			166.329	1.00 16.55	D	N
	ATOM	6403	CA	ASP	163	-8.711	-74.794	166.463	1.00 17.27	D	С
	ATOM	6404	СВ	ASP	163			167.434	1.00 18.34	D	C
	ATOM	6405	CG	ASP	163			168.853	1.00 20.38	D	С
	ATOM	6406	OD1	ASP	163			169.710	1.00 21.00	D	0
35	MOTA	6407	OD2	ASP	163			169.109	1.00 19.55	D	0
	MOTA	6408	С	ASP	163			165.168	1.00 16.59	D	С
	ATOM	6409	0	ASP	163	-9.773	-76.408	165.054	1.00 14.65	D	0
	MOTA	6410	N	ILE	164	-9.561	-74.351	164.196	1.00 15.61	D	N
	ATOM	6411	CA	ILE	164	-10.178	-74.802	162.955	1.00 15.63	D	С
40	MOTA	6412	CB	ILE	164	-10.877	-73.655	162.151	1.00 14.12	D	C
	ATOM	6413	CG2		164	-11.951	-73.003	163.018	1.00 15.01	D	С
	MOTA	6414	CG1	ILE	164	-9.857	-72.630	161.666	1.00 14.02	D	C
	MOTA	6415		ILE	164		-71.562	160.759	1.00 12.25	D	C
	MOTA	6416	С	ILE	164	-9.135	-75.494	162.081	1.00 16.00	D	С
45	MOTA	6417	0	ILE	164	-9.486	-76.288	3 161.215	1.00 16.41	D	0
	ATOM	6418	N	ASN	165	-7.855	-75.194	162.300	1.00 15.80	D	
	MOTA	6419	CA	ASN	165	-6.793	-75.851	161.542	1.00 17.21	D	C
	ATOM	6420	СВ	ASN	165	-5.421	-75.221	161.814	1.00 16.55	D	С
	ATOM	6421	CG	ASN	165	-5.211	-73.916	5 161.068	1.00 17.71	D	C
50	ATOM	6422	OD1	L ASN	165	-5.933	-73.603	3 160.122	1.00 16.40	D	0
	ATOM	6423		2 ASN	165	-4.198	-73.15	5 161.482	1.00 16.80	D	
	ATOM	6424		ASN	165	-6.763	-77.31	5 161.990	1.00 17.61	D	
	ATOM	6425		ASN	165			2 161.174		D	
	MOTA	6426		THR	166	-6.883	-77.53	9 163.297	1.00 17.61	D	
55	MOTA	6427	CA	THR	166	-6.893	3 -78.89	7 163.818			
	MOTA	6428		THR	166			7 165.355		D	
	MOTA	6429		1 THR				7 165.748	1.00 19.08		
	MOTA	6430		2 THR	166			1 165.927		D	

-280-

	MOTA	6431	С	THR	166			163.343	1.00 18.00		C
	ATOM	6432	0	THR	166			162.869	1.00 18.63		0
	MOTA	6433	N	PHE	167			163.462	1.00 17.77		N
_	MOTA	6434	CA	PHE	167	-10.569			1.00 18.33		C
5	ATOM	6435	CB	PHE	167	-11.700		163.157	1.00 18.78		C
	MOTA	6436	CG	PHE	167	-12.945			1.00 19.22		C
	MOTA	6437		PHE	167	-13.727		162.743	1.00 19.14		C
	MOTA	6438		PHE	167			161.294	1.00 19.37		C
40	MOTA	6439		PHE	167			162.036	1.00 18.14		С
10	MOTA	6440	CE2	PHE	167			160.583	1.00 19.96		C
	MOTA	6441	CZ	PHE	167	-15.279			1.00 20.10		C
	MOTA	6442	C	PHE	167			161.550	1.00 18.30	D	С
	MOTA	6443	0	PHE	167			161.211	1.00 18.49	D	0
45	MOTA	6444	N	MET	168			160.694	1.00 17.27	D	N
15	MOTA	6445	CA	MET	168			159.269	1.00 17.47	D	С
	MOTA	6446	CB	MET	168			158.484	1.00 17.11	D	C
	MOTA	6447	CG	MET	168			158.163	1.00 17.30	D	C
	MOTA	6448	SD	MET	168			157.061	1.00 15.92	D	S
00	MOTA	6449	CE	MET	168			158.216	1.00 15.99	D	C
20	ATOM	6450	C	MET	168			158.949	1.00 16.51	D	C
	MOTA	6451	0	MET	168			158.120	1.00 15.80	D	0
	ATOM	6452	N	VAL	169			159.582	1.00 16.26	D	N
	ATOM	6453	CA	VAL	169			159.313	1.00 17.34	D	C
25	ATOM	6454	CB	VAL	169			160.042	1.00 17.83	D	C
25	ATOM	6455		VAL	169			159.813	1.00 18.06	D	C
	ATOM	6456	CG2		169			159.527	1.00 17.43	D	C
	ATOM	6457	C	VAL	169		_	159.739	1.00 17.64	D	С
	ATOM	6458	0	VAL	169			159.076	1.00 16.56	D	0
30	ATOM	6459	N	LEU	170			160.847	1.00 17.79	D	N
30	ATOM	6460	CA	LEU	170			161.302	1.00 19.01	D	C
	ATOM	6461	CB CG	LEU	170			. 162.656 1 163.770	1.00 20.40 1.00 22.26	D D	C
	ATOM	6462		LEU LEU	170 170			2 165.038	1.00 22.26	D	C
	MOTA MOTA	6463 6464		LEU	170			164.010	1.00 23.21	D	C
35	ATOM	6465	CDZ	LEU	170			7 160.258	1.00 23.21	D	C
00	ATOM	6466	Ö	LEU	170			5 160.021	1.00 19.62	D	o
	ATOM	6467	N	GLN	171			159.621	1.00 19.02	D	N
	ATOM	6468	CA	GLN	171			5 158.591	1.00 19.08	D	C
	MOTA	6469	CB	GLN	171			5 158.225	1.00 19.14	D	Č
40	ATOM	6470	CG	GLN	171	-13.319		2 159.342	1.00 20.31	D	C
	ATOM	6471	CD	GLN	171			3 159.744	1.00 20.59	D	Č
	ATOM	6472		GLN	171			1 158.960	1.00 23.53	D	ō
	ATOM	6473	NE2	GLN	171			2 160.955	1.00 19.36	D	N
	ATOM	6474	C	GLN	171			4 157.346	1.00 19.36	D	C
45	ATOM	6475		GLN	171			1 156.736	1.00 18.90	D	Ō
. •	ATOM	6476		VAL	172			4 156.968	1.00 18.78	D	N
	ATOM	6477		VAL	172			9 155.817	1.00 19.25	D	C
	ATOM	6478		VAL	172			0 155.559	1.00 19.23	D	С
	ATOM	6479		1 VAL	172			2 154.527	1.00 17.92	D	C
50	ATOM	6480		2 VAL	172			7 155.063	1.00 18.09	D	C
	MOTA	6481		VAL	172			8 156.097	1.00 19.25	D	С
	ATOM	6482		VAL	172			0 155.213		D	0
	ATOM	6483		ILE	173			4 157.333		D	N
	ATOM	6484		ILE	173			7 157.748		D	С
55	ATOM	6485			173			8 159.227		D	С
	MOTA	6486		2 ILE	173			1 159.756	1.00 20.73		С
	ATOM	6487		1 ILE	173			6 159.332			С
	ATOM	6488		1 ILE	173			9 160.744			С

-281-

	MOTA	6489	С	ILE	173		-88.727		1.00 21.22	D	С
	MOTA	6490	0	ILE	173		-89.847		1.00 21.19	D	0
	MOTA	6491	N	LYS	174	-10.557			1.00 21.41	D	N
_	MOTA	6492	CA	LYS	174	-11.808			1.00 22.16	D	C
5	MOTA	6493	CB	LYS	174	-12.933			1.00 23.61	D	C
	MOTA	6494	CG	LYS	174	-12.720			1.00 25.13	D	C
	MOTA	6495	CD	LYS	174	-13.770			1.00 26.92	D	С
	MOTA	6496	CE	LYS	174	-15.122			1.00 30.21	D	C
40	MOTA	6497	NZ	LYS	174			161.705	1.00 31.50	D	N
10	MOTA	6498	C	LYS	174			156.348	1.00 22.88	D	C
	MOTA	6499	0	LYS	174			155.932	1.00 21.83	D	0
	MOTA	6500	N	PHE	175			155.548	1.00 23.02	D	N
	MOTA	6501	CA	PHE	175			154.107	1.00 23.18	D	С
4 =	ATOM	6502	СВ	PHE	175			153.498	1.00 22.95	D	С
15	MOTA	6503	CG	PHE	175			152.024	1.00 22.60	D	С
	MOTA	6504		PHE	175			151.086	1.00 21.67	D	C
	MOTA	6505		PHE	175			151.575	1.00 22.02	D	С
	MOTA	6506			175			149.719	1.00 22.60	D	С
	MOTA	6 507	CE2		175			150.215	1.00 22.13	D	С
20	MOTA	6508	CZ	PHE	175			149.284	1.00 22.45	D	C
	MOTA	6509	С	PHE	175			153.479	1.00 23.77	D	C
	MOTA	6510	0	PHE	175			152.725	1.00 23.33	D	0
	MOTA	6511	N	THR	176			153.805	1.00 24.37	D	N
05	MOTA	6512	CA	THR	176			153.248	1.00 25.40	D	C
25	MOTA	6513	СВ	THR	176			153.542	1.00 25.42	D	C
	MOTA	6514	OG1		176			154.956	1.00 26.76	D	0
	MOTA	6515	CG2		176			152.878	1.00 25.58	D	C
	MOTA	6516	С	THR	176			153.733	1.00 26.23	D	C
20	ATOM	6517	0	THR	176			153.012	1.00 26.27	D	0
30	MOTA	6518	N	LYS	177			154.935	1.00 26.44	D	N
	MOTA	6519	CA	LYS	177			155.453	1.00 27.74	D	С
	MOTA	6520	CB	LYS	177			156.867	1.00 27.72	D	С
	MOTA	6521	CG	LYS	177			157.354	1.00 28.98	D	C
25	MOTA	6522	CD	LYS	177			158.723	1.00 28.59	D	С
35	MOTA	6523	CE	LYS	177			159.106	1.00 28.79	D	C
	ATOM	6524	NZ	LYS	177			158.341	1.00 27.25	D	N
	MOTA	6525	C	LYS	177			154.546	1.00 27.56	D	C
	ATOM	6526	0	LYS	177			154.381	1.00 27.25	D	0
40	ATOM	6527	N	ASP	178			153.966	1.00 27.88	D	N
40	ATOM	6528	CA	ASP	178			153.069	1.00 28.74	D	C
	ATOM	6529	CB	ASP	178			153.006	1.00 29.09	D	C
	ATOM	6530	CG	ASP	178			154.258	1.00 30.01	D	_
	ATOM	6531		ASP	178			155.168	1.00 30.64	D	0
45	ATOM	6532		ASP	178			154.327	1.00 30.67	D	0
45	ATOM	6533	C	ASP	178			151.644	1.00 28.80	D	C
	ATOM	6534	0	ASP	178			150.743	1.00 29.46	D	0
	ATOM	6535	N	LEU	179			151.434	1.00 28.53	D	N
	ATOM	6536	CA	LEU	179			5 150.112	1.00 27.98 1.00 27.06	D	C
50	MOTA	6537	CB	LEU	179			2 149.696		D	
50	MOTA	6538	CG	LEU	179			5 149.737	1.00 26.57	D	
	MOTA	6539		LEU	179			3 149.145	1.00 26.43	D	
	MOTA	6540		2 LEU	179			5 148.959 2 150 105	1.00 25.98	D	
	ATOM	6541	C	LEU	179			3 150.185		D	
55	MOTA	6542 6543	0	LEU	179			2 150.683		D	-
33	ATOM	6543	N CD	PRO	180			5 149.682 7 149 999		D D	
	MOTA	6544	CD	PRO	180			7 148.999			
	ATOM	6545		PRO				7 149.691		D	_
	MOTA	6546	CB	PRO	180	-11.089	9 -98.71	3 148.793	1.00 29.68	D	С

-282-

	ATOM	6547	CG	PRO	180	-12.420	-98.052	149.056	1.00 28.81	D	С
	ATOM	6548	С	PRO	180	-8.691	-97.991	149.223	1.00 29.88	D	С
	ATOM	6549	0	PRO	180	-7.838	-98.543	149.918	1.00 29.69	D	0
	ATOM	6550	N	VAL	181	-8.399	-97.429	148.055	1.00 30.49	D	N
5	MOTA	6551	CA	VAL	181		-97.489		1.00 31.05	D	С
	ATOM	6552	CB	VAL	181		-96.959	146.105	1.00 32.32	D	C
	ATOM	6553	CG1		181			146.032	1.00 33.43	D	Ċ
	ATOM	6554	CG2		181			145.582	1.00 33.43	D	Č
	ATOM	6555	C	VAL	181			148.462	1.00 30.44	D	C
10	ATOM	6556	Ö	VAL	181			148.533	1.00 30.44	D	0
10	ATOM	6557		PHE	182			149.160	1.00 31.00		
			N							D	N
	ATOM	6558	CA	PHE	182			150.098	1.00 27.62	D	С
	MOTA	6559	CB	PHE	182			150.616	1.00 26.73	D	C
4 =	MOTA	6560	CG	PHE	182			151.645	1.00 26.35	D	C
15	MOTA	6561		PHE	182			151.256	1.00 26.19	D	С
	MOTA	6562	CD2	PHE	182			153.002	1.00 25.82	D	С
	MOTA	6563	CE1	PHE	182			152.204	1.00 25.18	Ð	С
	MOTA	6564	CE2	PHE	182			153.960	1.00 25.85	D	С
	MOTA	6565	CZ	PHE	182	-3.942	-91.599	153.558	1.00 24.75	D	С
20	ATOM	6566	C	PHE	182	-5.347	-96.000	151.273	1.00 27.26	D	С
	ATOM	6567	0	PHE	182	-4.218	-96.201	151.707	1.00 25.52	D	0
	ATOM	6568	N	ARG	183	-6.426	-96.599	151.772	1.00 27.61	D	N
	ATOM	6569	CA	ARG	183	-6.348	-97.535	152.900	1.00 29.82	D	С
	ATOM	6570	СВ	ARG	183			153.342	1.00 29.81	D	C
25	ATOM	6571	CG	ARG	183			153.834	1.00 30.04	D	C
	ATOM	6572	CD	ARG	183			155.126	1.00 31.16	D	Č
	ATOM	6573	NE	ARG	183			156.241	1.00 32.26	D	N
	ATOM	6574	CZ	ARG	183			156.752	1.00 33.84	Ď	C
	ATOM	6575	NH1		183			156.256	1.00 33.04	D	N
30	ATOM	6576	NH2		183			157.788	1.00 34.20	D	N
00	ATOM	6577	C	ARG	183			157.788			
								152.511	1.00 30.35	D	C
	ATOM	6578	0	ARG	183				1.00 30.29	D	0
	ATOM	6579	N	SER	184			151.335	1.00 30.53	D	N
35	ATOM	6580	CA	SER	184			150.937	1.00 31.20	D	C
35	ATOM	6581	CB	SER	184			149.472	1.00 31.90	D	C
	ATOM	6582	OG	SER	184			149.299	1.00 34.38	D	0
	ATOM	6583	C	SER	184			151.129	1.00 31.02	D	C
	ATOM	6584	0	SER	184			151.218	1.00 31.50	D	0
40	MOTA	6585	N	LEU	185			151.185	1.00 30.38	D	N
40	MOTA	6586	CA	LEU	185			151.369	1.00 30.35	D	C
	MOTA	6587	CB	LEU	185			151.031	1.00 30.07	D	C
	MOTA	6588	CG	LEU	185			149.683	1.00 30.04	D	C
	ATOM	6589		LEU	185			149.690	1.00 28.56	D	C
	MOTA	6590		LEU	185			148.546	1.00 28.92	D	С
45	ATOM	6591	С	LEU	185			7 152.831	1.00 30.64	D	С
	ATOM	6592	0	LEU	185			2 153.696	1.00 30.76	D	0
	MOTA	6593	N	PRO	186	0.320	-99.018	3 153.125	1.00 31.27	D	N
	ATOM	6594	CD	PRO	186	1.483	-99.091	l 152.224	1.00 31.66	D	C
	ATOM	6595	CA	PRO	186	0.724	-99.235	5 154.515	1.00 31.60	D	C
50	MOTA	6596	СВ	PRO	186	2.220	-99.522	2 154.401	1.00 31.16	D	C
	MOTA	6597	CG	PRO	186			153.164	1.00 32.29	D	C
	ATOM	6598	C	PRO	186			5 155.299	1.00 31.66	D	C
	ATOM	6599	ō	PRO	186			5 154.791	1.00 31.55	D	Ö
	ATOM	6600		ILE	187			5 154.731	1.00 31.45	D	N
55	MOTA	6601	CA	ILE	187	-0.425		9 157.351	1.00 31.45	D	C
	MOTA	6602		ILE	187			7 158.766			C
	ATOM	6603		ILE					1.00 29.37	D	
								9 159.591			C
	MOTA	6604	CG.	LILE	187	-1.606	96.26	4 159.476	1.00 28.40	D	C

-283-

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	ATOM	6605	CD1		187		-96.690		1.00 27.64	D	C
	ATOM	6606	C	ILE	187		-95.861		1.00 31.86	D	C
	ATOM	6607	0	ILE	187		-94.683		1.00 31.41	D	0
_	ATOM	6608	N	GLU	188		-96.220		1.00 32.22	D	N
5	ATOM	6609	CA	GLU	188		-95.207		1.00 33.67	D	C
	ATOM	6610	СВ	GLU	188		-95.847		1.00 35.42	D	C
	ATOM	6611	CG	GLU	188			156.663	1.00 38.74	D	С
	ATOM	6612	CD	GLU	188			156.936	1.00 41.52	D	C
40	MOTA	6613		GLU	188			157.118	1.00 42.54	D	0
10	MOTA	6614		GLU	188			156.974	1.00 42.40	D	0
	MOTA	6615	С	GLU	188			156.307	1.00 33.32	D	C
	MOTA	6616	0	GLU	188			156.381	1.00 33.14	D	0
	MOTA	6617	N	ASP	189			155.163	1.00 32.68	D	N
4.5	MOTA	6618	CA	ASP	189			153.921	1.00 32.83	D	С
15	MOTA	6619	CB	ASP	189			152.713	1.00 35.38	D	C
	MOTA	6620	CG	ASP	189			152.465	1.00 37.57	D	С
	MOTA	6621		ASP	189			153.384	1.00 40.86	D	0
	MOTA	6622		ASP	189			151.354	1.00 37.64	D	0
	MOTA	6623	C	ASP	189			153.986	1.00 30.96	D	С
20	MOTA	6624	0	ASP	189			153.588	1.00 30.94	D	0
	MOTA	6625	N	GLN	190	0.262	-93.786	154.494	1.00 29.38	D	N
	MOTA	6626	CA	GLN	190	-0.973	-93.024	154.632	1.00 28.01	D	C
	MOTA	6627	CB	GLN	190	-2.046	-93.857	155.350	1.00 28.17	D	С
	ATOM	6628	CG	GLN	190	-2.416	-95.171	154.661	1.00 28.90	D	С
25	ATOM	6629	CD	GLN	190	-3.592	-95.899	155.323	1.00 29.16	D	С
	MOTA	6630	OE1	GLN	190	-3.808	-97.093	155.094	1.00 29.27	D	0
	MOTA	6631	NE2	GLN	190	-4.359	-95.180	156.130	1.00 28.27	D	N
	MOTA	6632	C	GLN	190	-0.675	-91.765	155.447	1.00 27.34	D	С
	ATOM	6633	0	GLN	190	-1.122	-90.667	155.110	1.00 25.56	D	0
30	MOTA	6634	N	ILE	191	0.089	-91.935	156.523	1.00 26.72	D	N
	MOTA	6635	CA	ILE	191			157.389	1.00 26.98	D	C
	ATOM	6636	CB	ILE	191	1.106	-91.337	158.693	1.00 27.03	D	С
	MOTA	6637	CG2	ILE	191	1.671	-90.168	159.487	1.00 26.61	D	С
	MOTA	6638	CG1	ILE	191	0.066	-92.108	159.520	1.00 26.71	D	С
35	MOTA	6639	CD1	ILE	191			160.693	1.00 27.05	D	C
	MOTA	6640	C	ILE	191	1.396	-89.835	156.690	1.00 26.93	D	C
	MOTA	6641	0	ILE	191	1.261	-88.624	156.859	1.00 25.97	D	0
	MOTA	6642	N	SER	192	2.343	-90.348	155.907	1.00 25.82	D	N
	ATOM	6643	CA	SER	192	3.270	-89.486	155.183	1.00 26.80	D	C
40	ATOM	6644	CB	SER	192	4.338	-90.325	154.473	1.00 27.15	D	C
	MOTA	6645	OG	SER	192	5.203	-90.939	155.415	1.00 29.76	D	0
	MOTA	6646	С	SER	192	2.531	-88.623	154.154	1.00 25.97	D	C
	MOTA	6647	0	SER	192	2.788	-87.425	154.037	1.00 25.52	D	0
	MOTA	6648	N	LEU	193	1.621	-89.238	153.407	1.00 24.97	D	N
45	MOTA	6649	CA	LEU	193	0.857	-88.516	152.402	1.00 24.60	D	C
	MOTA	6650	CB	LEU	193	0.061	-89.495	151.539	1.00 24.47	D	C
	MOTA	6651	CG	LEU	193	0.866	-90.473	150.667	1.00 25.09	D	C
	MOTA	6652	CD1	LEU	193	-0.091	-91.410	149.936	1.00 21.73	D	C
	ATOM	6653	CD2	LEU	193	1.740	-89.688	3 149.673	1.00 24.35	D	C
50	MOTA	6654	С	LEU	193	-0.088	-87.488	3 153.032	1.00 24.39	D	С
	MOTA	6655	0	LEU	193	-0.296	-86.410	152.476	1.00 23.01	D	0
	MOTA	6656	N	LEU	194			154.181	1.00 24.06	D	N
	MOTA	6657	CA	LEU	194			5 154.862	1.00 24.67	D	C
	MOTA	6658	CB	LEU	194			1 156.014		D	C
55	ATOM	6659	CG	LEU	194			2 155.880		D	C
_	ATOM	6660		LEU	194			2 156.161		D	Č
	ATOM	6661		2 LEU	194			7 154.492		D	Č
	ATOM	6662		LEU	194			1 155.375		D	C
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PCT/US2004/023092

	MOTA	6663	0	LEU	194	-1.173	-84.559	155.227	1.00 24.50	D	0
	MOTA	6664	N	LYS	195	0.397	-85.999	155.949	1.00 24.56	D	N
	ATOM	6665	CA	LYS	195	1.287	-84.971	156.462	1.00 25.60	D	C
_	ATOM	6666	CB	LYS	195	2.513	-85.642	157.085	1.00 26.77	D	C
5	ATOM	6667	CG	LYS	195	3.439	-84.704	157.827	1.00 31.05	D	C
	ATOM	6668	CD	LYS	195	4.510	-85.476	158.608	1.00 33.47	D	С
	ATOM	6669	CE	LYS	195	5.494	-86.190	157.686	1.00 34.73	D	C
	ATOM	6670	NZ	LYS	195	6.494	-87.008	158.448	1.00 37.37	D	N
	ATOM	6671	С	LYS	195	1.715	-83.990	155.349	1.00 24.73	D	С
10	ATOM	6672	0	LYS	195	1.796	-82.776	155.569	1.00 23.70	D	0
	ATOM	6673	N	GLY	196	1.967	-84.513	154.152	1.00 22.84	D	N
	ATOM	6674	CA	GLY	196	2.386	-83.652	153.062	1.00 21.25	D	С
	ATOM	6675	С	GLY	196	1.284	-82.952	152.282	1.00 20.83	D	С
	MOTA	6676	0	GLY	196	1.511	-81.894	151.705	1.00 20.29	D	0
15	ATOM	6677	N	ALA	197			152.277	1.00 20.54	D	N
	ATOM	6678	CA	ALA	197		-82.932		1.00 19.62	D	C
	ATOM	6679	СВ	ALA	197		-83.983		1.00 18.07	D	С
	ATOM	6680	C	ALA	197		-82.320		1.00 18.74	D	C
	ATOM	6681	ō	ALA	197			151.634	1.00 17.93	D	Ō
20	ATOM	6682	N	ALA	198			153.542	1.00 18.19	D	N
	ATOM	6683	CA	ALA	198			154.311	1.00 17.94	D	c
	ATOM	6684	СВ	ALA	198			155.805	1.00 18.85	D	Č
	ATOM	6685	C	ALA	198			154.102	1.00 16.59	D	Č
	ATOM	6686	Ö	ALA	198			153.758	1.00 15.86	D	ŏ
25	ATOM	6687	N	VAL	199			154.320	1.00 16.08	D	N
	ATOM	6688	CA	VAL	199			154.142	1.00 16.51	D	C
	ATOM	6689	СВ	VAL	199			154.467	1.00 16.75	Ď	č
	ATOM	6690	_	VAL	199			154.138	1.00 18.24	D	Č
	ATOM	6691		VAL	199			155.945	1.00 18.67	D	c
30	ATOM	6692	C	VAL	199			152.709	1.00 16.12	D	C
00	ATOM	6693	Ö	VAL	199			152.498	1.00 14.02	D	ŏ
	ATOM	6694	N	GLU	200			151.727	1.00 15.48	D	N
	ATOM	6695	CA	GLU	200			150.330	1.00 16.73	D	C
	ATOM	6696	CB	GLU	200			149.417	1.00 16.75	D	C
35	ATOM	6697	CG	GLU	200			149.252	1.00 10.30	D	C
00	ATOM	6698	CD	GLU	200			148.533	1.00 17.00	D	Č
	ATOM	6699		GLU	200			140.533	1.00 19.22	D	Ö
	MOTA	6700	OE2		200			148.975	1.00 20.12	D	Ö
	ATOM	6701	C	GLU	200			150.035	1.00 15.98	D	c
40		6702	0	GLU	200			L 149.402	1.00 15.85	D	0
40	ATOM ATOM	6702	N	ILE	201	-4.989		150.499	1.00 15.63	D	N
	ATOM	6704	CA	ILE	201			150.499	1.00 15.51	D	C
		6705	_		201			3 150.233	1.00 15.91	D	
	ATOM		CB CG2	ILE	201			150.927	1.00 15.40	D	C
45	ATOM	6706									
40	ATOM	6707		ILE	201			3 150.129 1 150.870	1.00 18.12	D D	C
	ATOM	6708		ILE	201			7 150.875	1.00 15.80	D	C
	ATOM	6709		ILE	201				1.00 15.21		
	MOTA	6710		ILE	201			7 150.251	1.00 14.04	D	0
50	ATOM	6711		CYS	202			2 152.119	1.00 14.29	D	N
50	MOTA	6712		CYS	202			7 152.776		D	C
	ATOM	6713		CYS	202			4 154.155	1.00 14.22	D	C
	ATOM	6714		CYS	202			2 155.348		D	S
	MOTA	6715		CYS	202			9 151.931	1.00 14.68	D	C
	MOTA	6716		CYS	202			0 151.809			0
55	MOTA	6717		HIS	203			3 151.343			N
	MOTA	6718		HIS	203			4 150.509			_
	MOTA	6719		HIS				6 150.140			C
	MOTA	6720	CG	HIS	203	-5.186	5 -73.58	8 151.227	1.00 16.92	D	C

-285-

	MOTA	6721	CD2 HIS	203	-4.115	-73.810	152 024	1.00 17.06	D	С
	ATOM	6722	ND1 HIS	203		-72.389		1.00 17.22	D	N
	ATOM	6723	CE1 HIS	203		-71.905		1.00 17.22	D	C
	ATOM	6724	NE2 HIS	203			152.893	1.00 17.67	D	N
5	ATOM	6725	C HIS	203		-75.249	149.261	1.00 15.18	D	C
·	MOTA	6726	O HIS	203		-74.395		1.00 13.18	D	Ö
	MOTA	6727	N ILE	204		-76.441		1.00 15.83	D	N
	ATOM	6728	CA ILE	204		-76.797		1.00 15.89	D	C
	ATOM	6729	CB ILE	204		-78.195		1.00 16.42	D	C
10	ATOM	6730	CG2 ILE	204		-78.664		1.00 15.76	D	C
10	ATOM	6731	CG2 ILE	204		-78.148		1.00 15.76		C
	ATOM	6732	CD1 ILE	204		-79.496		1.00 18.43	D D	C
		6733		204	-10.108					C
	MOTA	6734		204			147.895	1.00 16.28 1.00 15.45	D	
15	MOTA				-10.943				D	0
15	MOTA	6735	N VAL	205	-10.423		149.043	1.00 15.70	D	N
	ATOM	6736	CA VAL	205	-11.799			1.00 16.11	D	C
	ATOM	6737	CB VAL	205	-11.895		150.759	1.00 16.88	D	C
	ATOM	6738	CG1 VAL	205	-13.274		151.427	1.00 16.36	D	C
20	ATOM	6739	CG2 VAL	205			150.315	1.00 16.38	D	C
20	ATOM	6740	C VAL	205			149.906	1.00 16.68	D	С
	ATOM	6741	O VAL	205			149.545	1.00 16.11	D	0
	MOTA	6742	N LEU	206			150.635	1.00 16.97	D	N
	ATOM	6743	CA LEU	206			151.057	1.00 18.74	D	C
25	ATOM	6744	CB LEU	206				1.00 19.59	D	C
25	ATOM	6745	CG LEU	206			153.491	1.00 21.97	D	C
	ATOM	6746	CD1 LEU	206			153.922	1.00 23.35	D	C
	ATOM	6747	CD2 LEU	206			154.403	1.00 22.61	D	C
	MOTA	6748	C LEU	206			149.886	1.00 18.61	D	C
20	MOTA	6749	O LEU	206			150.023	1.00 18.78	D	0
30	MOTA	6750	n asn	207			148.740	1.00 17.84	D	N
	ATOM	6751	CA ASN	207			147.569	1.00 18.81	D	С
	MOTA	6752	CB ASN	207			146.358	1.00 16.45	D	C
	MOTA	6753	CG ASN	207			145.167	1.00 17.11	D	C
25	MOTA	6754	OD1 ASN	207			144.162	1.00 13.45	D	0
35	ATOM	6755	ND2 ASN	207			145.283	1.00 15.61	D	N
	MOTA	6756	C ASN	207			147.206	1.00 19.76	D	С
	MOTA	6757	O ASN	207			146.727	1.00 19.75	D	0
	ATOM	6758	N THR				147.442	1.00 20.34	D	N
40	MOTA	6759	CA THR				147.111	1.00 22.21	D	С
40	MOTA	6760	CB THR				147.240	1.00 23.45	D	С
	MOTA	6761	OG1 THR				148.599	1.00 23.83	D	0
	MOTA	6762	CG2 THR				146.332	1.00 24.88	D	C
	MOTA	6763	C THR				147.938	1.00 21.89	D	С
AE	MOTA	6764	O THR				147.626	1.00 23.81	D	0
45	MOTA	6765	N THR				148.981	1.00 20.43	D	N
	MOTA	6766	CA THR				149.799	1.00 19.96	D	C
	MOTA	6767	CB THR				151.320	1.00 18.96	D	C
	MOTA	6768	OG1 THR				151.632	1.00 17.92	D	0
	MOTA	6769	CG2 THR				151.732	1.00 18.80	D	С
50	MOTA	6770					. 149.455	1.00 19.40	D	С
	MOTA	6771					150.008	1.00 19.55	D	0
	MOTA	6772					148.544		D	N
	MOTA	6773					148.151	1.00 20.20	D	С
	ATOM	6774					147.433	1.00 19.49	D	С
55	MOTA	6775					147.289		D	С
	ATOM	6776					2 148.396		D	C
	ATOM	6777					7 146.046		D	C
	MOTA	6778	CE1 PHE	210	-10.054	-65.350	148.265	1.00 17.81	D	С

-286-

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	ATOM	6779	CE2		210	-10.500			1.00 17.22		C
	ATOM	6780	CZ	PHE	210		-64.775		1.00 18.25		C
	MOTA	6781	C	PHE	210	-14.722			1.00 21.26	D	C
5 .	ATOM	6782	0	PHE	210	-15.199			1.00 20.72	D	0
3 .	ATOM	6783	N	CYS	211	-14.926			1.00 23.14	D	N
	MOTA	6784	CA	CYS	211	-15.736			1.00 25.64	D	C
	ATOM	6785	CB	CYS	211	-16.594			1.00 26.00	D	C
	ATOM	6786	SG	CYS	211	-17.553			1.00 28.41	D	S
10	ATOM	6787	C	CYS	211	-14.812			1.00 27.00	D	C
10	ATOM	6788	0	CYS	211	-14.064			1.00 26.49	D	0
	ATOM	6789	N	LEU	212	-14.865			1.00 28.64	D	N
	MOTA	6790	CA	LEU	212	-14.032			1.00 30.45	D	C
	MOTA	6791	CB	LEU	212		-63.683		1.00 30.47	D	C
4 5	MOTA	6792	CG	LEU	212		-65.084		1.00 30.70	D	C
15	MOTA	6793		LEU	212		-65.364		1.00 31.20	D	C
	ATOM	6794		LEU	212		-65.183		1.00 30.24	D	C
	MOTA	6795	C	LEU	212		-61.748		1.00 31.68	D	C
	MOTA	6796	0	LEU	212		-60.964		1.00 31.74	D	0
00	MOTA	6797	N	GLN	213		-61.349		1.00 32.60	D	N
20	MOTA	6798	CA	GLN	213		-59.935		1.00 33.45	D	С
	MOTA	6799	CB	GLN	213		-59.763		1.00 36.26	D	С
	MOTA	6800	CG	GLN	213		-58.346		1.00 40.79	D	C
	MOTA	6801	CD	GLN	213		-58.213		1.00 43.35	D	C
0.5	MOTA	6802	OE1		213		-58.316		1.00 44.82	D	0
25	MOTA	6803	NE2		213		-57.984		1.00 44.19	D	N
	MOTA	6804	С	GLN	213		-59.209		1.00 32.04	D	С
	MOTA	6805	0	GLN	213		-58.067		1.00 31.86	D	0
	MOTA	6806	N	THR	214			146.629	1.00 30.21	D	N
00	MOTA	6807	CA	THR	214			147.803	1.00 28.64	D	С
30	MOTA	6808	CB	THR	214			149.002	1.00 28.97	D	С
	MOTA	6809	OG1		214			149.218	1.00 28.69	D	0
	MOTA	6810		THR	214			148.736	1.00 28.63	D	C
	MOTA	6811	С	THR	214			148.253	1.00 27.89	D	С
0.5	MOTA	6812	0	THR	214			149.184	1.00 27.24	D	0
35	MOTA	6813	N	GLN	215			147.600	1.00 27.59	D	N
	MOTA	6814	CA	GLN	215			147.969	1.00 27.84	D	С
	MOTA	6815	CB	GLN	215			147.836	1.00 29.73	D	C
	MOTA	6816	CG	GLN	215			146.458	1.00 32.60	D	C
40	MOTA	6817	CD	GLN	215			145.407	1.00 34.25	D	C
40	MOTA	6818	OE1		215			144.550	1.00 36.19	D	0
	ATOM	6819		GLN	215			145.471	1.00 35.54	D	N
	ATOM	6820	С	GLN	215			149.419	1.00 26.63	D	C
	MOTA	6821	0	GLN	215			150.158	1.00 25.86	D	0
45	MOTA	6822	N	ASN	216			149.810	1.00 25.65	D	N
45	MOTA	6823	CA	ASN	216			151.160	1.00 25.70	D	C
	ATOM	6824	CB	ASN	216			151.812	1.00 27.21	D	C
	MOTA	6825	CG	ASN	216			152.208	1.00 29.76	D	С
	MOTA	6826		LASN	216			152.492	1.00 31.19	D	0
	MOTA	6827		2 ASN	216			152.258	1.00 31.91	D	N
50	MOTA	6828		ASN	216			151.133	1.00 24.52	D	С
	ATOM	6829		ASN	216			150.103	1.00 23.28	D	0
	ATOM	6830		PHE	217			152.276	1.00 23.35	D	N
	MOTA	6831		PHE	217			152.396	1.00 22.98	D	C
FF	ATOM	6832		PHE	217			153.131	1.00 20.37	D	С
55	ATOM	6833		PHE	217			152.352	1.00 19.81	D	C
	MOTA	6834		1 PHE	217			152.396	1.00 19.27		С
	MOTA	6835		2 PHE	217			151.556	1.00 19.27		-
	MOTA	6836	CE	1 PHE	217	-9.291	-67.043	3 151.655	1.00 19.72	D	C

-287-

	MOTA	6837	CE2	PHE	217	-10.228	-69.088	150.811	1.00 19.86	D	C
	ATOM	6838	CZ	PHE	217	-9.177	-68.176	150.862	1.00 19.40	D	С
	ATOM	6839	С	PHE	217	-15.094	-66.486	153.211	1.00 23.95	D	C
_	ATOM	6840	0	PHE	217	-15.074	-66.063	154.370	1.00 23.31	D	0
5	ATOM	6841	N	LEU	218	-16.216	-66.839	152.591	1.00 24.22	D	N
	ATOM	6842	CA	LEU	218	-17.508	-66.776	153.261	1.00 25.10	D	C
	MOTA	6843	CB	LEU	218	-18.586	-66.298	152.286	1.00 26.14	D	C
	ATOM	6844	CG	LEU	218	-18.260	-64.972	151.583	1.00 27.28	D	С
	MOTA	6845	CD1	LEU	218	-19.386	-64.588	150.624	1.00 26.98	D	С
10	MOTA	6846	CD2	LEU	218	-18.041	-63.883	152.640	1.00 27.40	D	С
	ATOM	6847	С	LEU	218		-68.163		1.00 25.53	D	C
	MOTA	6848	0	LEU	218		-69.087		1.00 25.80	D	Ö
	ATOM	6849	N	CYS	219			155.103	1.00 25.26	D	N
	ATOM	6850	CA	CYS	219		-69.588		1.00 25.79	D	C
15	ATOM	6851	CB	CYS	219		-70.044		1.00 25.11	D	Ċ
	ATOM	6852	SG	CYS	219			155.391	1.00 24.90	D	s
	ATOM	6853	C	CYS	219			156.674	1.00 25.79	Ď	c
	ATOM	6854	ŏ	CYS	219			157.857	1.00 25.32	D	ŏ
	ATOM	6855	N	GLY	220			156.131	1.00 25.40	D	N
20	ATOM	6856	CA	GLY	220			156.922	1.00 24.69	D	C
	ATOM	6857	C	GLY	220			157.341	1.00 24.74	D	C
	ATOM	6858	Ö	GLY	220			156.492	1.00 24.74	D	o
	MOTA	6859	N	PRO	221			158.649	1.00 24.33	D	N
	ATOM	6860	CD	PRO	221			159.758	1.00 24.44	D	C
25	MOTA	6861	CA	PRO	221			159.738	1.00 24.10	D	C
	ATOM	6862	СВ	PRO	221			160.495	1.00 24.43	D	C
	MOTA	6863	CG	PRO	221			160.493	1.00 23.03		C
	ATOM	6864	C	PRO	221			159.192	1.00 24.72	D	C
	ATOM	6865	Ö	PRO	221			159.192	1.00 24.14	D	0
30	ATOM	6866	N	LEU	222			159.401	1.00 24.82	D	И
00	ATOM	6867	CA	LEU	222					D	
	ATOM	6868	CB	LEU	222			159.097	1.00 22.19	D	C
	ATOM	6869	CG	LEU	222			159.675	1.00 20.44	D	C
	ATOM	6870		LEU				160.991	1.00 19.18	D	C
35	ATOM	6871		LEU	222 222			161.478	1.00 18.47	D	C
00								162.031	1.00 17.33	D	C
	MOTA	6872	C	LEU	222			157.771	1.00 21.62	D	C
	MOTA ATOM	6873 6874	0	LEU	222			156.697	1.00 21.70	D	0
			N	ARG	223 223			157.871	1.00 21.04	D	N
40	MOTA	6875	CA	ARG				156.709	1.00 21.51	D	C
40	ATOM	6876	CB	ARG	223			156.424	1.00 22.86	D	C
	ATOM	6877	CG	ARG	223			155.282	1.00 25.93	D	C
	ATOM	6878	CD	ARG	223			155.770	1.00 27.48	D	С
	ATOM	6879	NE	ARG	223			156.520	1.00 28.36	D	N
45	MOTA	6880	CZ	ARG	223			157.850	1.00 29.02	D	С
45	MOTA	6881		ARG	223			158.613	1.00 28.03	D	N
	ATOM	6882		ARG	223			158.425	1.00 28.61	D	N
	ATOM	6883	C	ARG	223			157.043	1.00 20.57	D	C
	MOTA	6884	0	ARG	223			157.889	1.00 20.75	D	0
E 0	ATOM	6885	N	TYR	224			156.407	1.00 18.81	D	N
50	ATOM	6886	CA	TYR	224			156.640	1.00 17.92	D	C
	MOTA	6887	СВ	TYR	224			156.654	1.00 17.02	D	С
	ATOM	6888	CG	TYR	224			157.744	1.00 17.15	D	С
	MOTA	6889	CD1		224			157.530	1.00 17.59	D	C
	ATOM	6890	CE1		224			158.524	1.00 17.94	D	С
55	MOTA	6891	CD2		224			158.981	1.00 15.66	D	C
	MOTA	6892	CE2		224			159.985	1.00 16.21	D	C
	MOTA	6893	CZ	TYR				159.749	1.00 16.87	D	С
	MOTA	6894	OH	TYR	224	-13.512	-69.256	160.725	1.00 15.77	D	0

-288-

	MOTA	6895	C	TYR	224	-11.609			1.00 17.55		C
	MOTA	6896	0	TYR	224	-11.878			1.00 16.13		0
	MOTA	6897	N	THR	225	-10.718	-62.638	155.972	1.00 16.25	_	N
_	MOTA	6898	CA	THR	225	-10.022			1.00 16.87		C
5	MOTA	6899	CB	THR	225	-10.325			1.00 17.79		C
	ATOM	6900	OG1	THR	225		-59.964		1.00 17.11		0
	ATOM	6901	CG2	THR	225	-11.827	-59.993	155.348	1.00 18.41		C
	ATOM	6902	C	THR	225	-8.505	-61.926	155.098	1.00 16.77		C
	MOTA	6903	0	THR	225		-62.593		1.00 15.99		0
10	MOTA	6904	N	ILE	226		-61.287		1.00 16.23		N
	MOTA	6905	CA	ILE	226		-61.354		1.00 16.57	D	C
	MOTA	6906	CB	ILE	226	-5.859		152.769	1.00 17.02	D	C
	MOTA	6907	CG2	ILE	226		-59.202		1.00 15.14	D	C
	MOTA	6908	CG1	ILE	226		-61.149		1.00 16.61	D	С
15	ATOM	6909	CD1	ILE	226			151.185	1.00 14.79	D	C
	ATOM	6910	С	ILE	226			155.327	1.00 17.24	D	C
	ATOM	6911	0	ILE	226			155.751	1.00 16.91	D	0
	MOTA	6912	N	GLU	227			155.919	1.00 16.07	D	N
	MOTA	6913	CA	GLU	227			157.103	1.00 16.95	D	C
20	MOTA	6914	CB	GLU	227			157.495	1.00 16.63	D	C
	MOTA	6915	CG	GLU	227	-6.820	-56.578	156.571	1.00 16.07	D	C
	ATOM	6916	CD	GLU	227			155.195	1.00 16.66	D	C
	MOTA	6917	OE1	GLU	227		-57.443		1.00 16.07	D	0
	ATOM	6918	OE2	GLU	227			154.187	1.00 17.97	D	0
25	MOTA	6919	С	GLU	227	•		158.280	1.00 16.47	D	С
	MOTA	6920	0	GLU	227			159.159	1.00 16.40	D	0
	MOTA	6921	N	ASP	228			158.309	1.00 15.66	D	N
	MOTA	6922	CA	ASP	228			159.393	1.00 16.51	D	C
	MOTA	6923	CB	ASP	228			159.311	1.00 15.72	D	С
30	MOTA	6924	CG	ASP	228			159.555	1.00 16.63	D	С
	MOTA	6925	-	ASP	228			160.540	1.00 16.26	D	0
	MOTA	6926	OD2	ASP	228			158.768	1.00 16.57	D	0
	MOTA	6927	С	ASP	228			159.361	1.00 15.84	D	С
~ -	MOTA	6928	0	ASP	228			160.406	1.00 17.26	D	0
35	MOTA	6929	N	GLY	229			158.164	1.00 15.54	D	N
	ATOM	6930	CA	GLY	229			158.053	1.00 14.97	D	C
	MOTA	6931	С	GLY	229			158.385	1.00 15.19	D	C
	MOTA	6932	0	GLY	229			159.010	1.00 14.72	D	0
40	MOTA	6933	N	ALA	230			157.973	1.00 13.93	D	N
40	MOTA	6934	CA	ALA	230			158.233	1.00 14.50	D	C
	MOTA	6935	СВ	ALA	230			157.456	1.00 14.94	D	C
	MOTA	6936		ALA	230			3 159.732	1.00 14.36	D	C
	MOTA	6937		ALA	230			160.263	1.00 12.75	D	0
AF	MOTA	6938		ARG	231			160.410	1.00 14.18	D	И
45	ATOM	6939		ARG	231			7 161.840	1.00 15.32	D	C
	MOTA	6940		ARG	231			4 162.324	1.00 15.52	D	C
	MOTA	6941		ARG	231			B 161.761		D	C
	MOTA	6942		ARG	231			8 162.224		D	C
ΕO	MOTA	6943		ARG	231			7 163.665		D	N
50	MOTA	6944		ARG	231			4 164.246		D D	C
	MOTA	6945		1 ARG	231			0 163.527			N
	ATOM	6946		2 ARG	231			9 165.559		D	N
	ATOM	6947		ARG	231			6 162.698		D	C
EE	ATOM	6948		ARG	231			1 163.805			0
55	ATOM	6949		VAL	232			1 162.220			
	ATOM	6950			232			9 163.038			
	MOTA	6951			232			0 162.869			_
	MOTA	6952	: CG	1 VAL	232	-3.73	0 -04.51	4 163.233	1.00 17.47	ט	Ċ

-289-

	MOTA	6953	CG2		232		-65.247		1.00 16.56	D	C
	MOTA	6954		VAL	232		-63.552		1.00 15.66	D	C
	MOTA	6955	0	VAL	232	0.607	-64.442	163.302	1.00 14.93	D	0
_	MOTA	6956	N	GLY	233			161.868	1.00 15.13	D	N
5	ATOM	6957	CA	GLY	233	1.946	-62.818	161.586	1.00 15.93	D	C
	MOTA	6958	С	GLY	233	2.433	-63.251	160.218	1.00 16.55	D	С
	ATOM	6959	0	GLY	233	3.630	-63.157	159.961	1.00 16.84	D	0
	MOTA	6960	N	PHE	234	1.555	-63.741	159.347	1.00 16.39	D	N
	MOTA	6961	CA	PHE	234			158.017	1.00 17.11	D	С
10	ATOM	6962	СВ	PHE	234			157.226	1.00 16.36	D	C
	ATOM	6963	CG	PHE	234			157.703	1.00 16.05	D	C
	ATOM	6964	CD1		234			158.386	1.00 14.44	D	Č
	ATOM	6965	CD2		234			157.420	1.00 15.78	D	Č
	ATOM	6966		PHE	234			158.779	1.00 16.61	D	Ċ
15	MOTA	6967		PHE	234			157.807	1.00 15.23	D	C
	ATOM	6968	CZ	PHE	234			158.486	1.00 15.25	D	C
	MOTA	6969	C	PHE	234			157.234	1.00 13.09	D	C
	MOTA	6970	0	PHE	234			157.234	1.00 18.10	D	0
								156.451			
20	ATOM	6971	N	GLN	235				1.00 19.12	D	N
20	ATOM	6972	CA	GLN	235			155.624	1.00 19.59	D	C
	MOTA	6973	CB	GLN	235			155.052	1.00 21.47	D	C
	MOTA	6974	CG	GLN	235			156.080	1.00 25.04	D	C
	ATOM	6975	CD	GLN	235			155.433	1.00 27.60	D	C
0E	MOTA	6976	OE1		235			154.643	1.00 28.65	D	0
25	MOTA	6977	NE2	GLN	235			155.760	1.00 28.31	D	N
	MOTA	6978	С	GLN	235			154.476	1.00 19.54	D	С
	MOTA	6979	0	GLN	235			153.920	1.00 18.79	D	0
	MOTA	6980	N	VAL	236			154.119	1.00 19.32	D	N
	MOTA	6981	CA	VAL	236			153.053	1.00 19.50	D	С
30	MOTA	6982	CB	VAL	236			152.866	1.00 19.33	D	С
	ATOM	6983		VAL	236			151.660	1.00 18.53	D	С
	MOTA	6984	CG2	VAL	236	1.577	-57.913	154.126	1.00 18.96	D	C
	MOTA	6985	С	VAL	236	2.294	-60.806	151.708	1.00 19.71	D	C
	MOTA	6986	0	VAL	236	1.352	-61.243	151.058	1.00 19.46	D	0
35	MOTA	6987	N	GLU	237	3.551	-60.888	151.287	1.00 20.19	D	N
	MOTA	6988	CA	GLU	237	3.892	-61.523	150.014	1.00 21.32	D	С
	MOTA	6989	CB	GLU	237	5.407	-61.463	149.802	1.00 23.35	D	С
	MOTA	6990	CG	GLU	237	5.888	-62.029	148.485	1.00 27.69	D	C
	MOTA	6991	CD	GLU	237	7.288	-61.544	148.135	1.00 31.29	D	C
40	MOTA	6992	OE1	GLU	237	7.435	-60.350	147.778	1.00 33.68	D	0
	MOTA	6993	OE2	GLU	237	8.239	-62.346	148.229	1.00 32.41	D	0
	MOTA	6994	С	GLU	237	3.396	-62.975	149.960	1.00 20.15	D	С
	ATOM	6995	0	GLU	237	2.873	-63.428	148.942	1.00 19.45	D	0
	ATOM	6996	N	PHE	238			151.061	1.00 18.94	D	N
45	ATOM	6997	CA	PHE	238	3.110		5 151.152	1.00 18.95	D	C
	MOTA	6998	СВ	PHE	238			152.511	1.00 18.87	D	C
	MOTA	6999	CG	PHE	238			2 152.862	1.00 18.24	D	Ċ
	ATOM	7000		PHE	238			2 152.239	1.00 18.39	D	Č
	ATOM	7001		PHE	238	1.769		153.797	1.00 18.85	D	c
50	ATOM	7002		PHE	238			7 152.545	1.00 18.05	D	c
00	ATOM	7002	CE2		238			9 154.109	1.00 10.03	D	c
	ATOM	7003	CZ	PHE	238			153.480	1.00 18.89	D	C
										D	
	ATOM	7005	C	PHE	238			150.998	1.00 19.39		C
55	ATOM	7006	0	PHE	238			4 150.239	1.00 18.49	D	0
J	ATOM	7007		LEU	239			3 151.713	1.00 18.74	D	N
	ATOM	7008		LEU	239			6 151.675	1.00 19.82	D	C
	ATOM	7009		LEU	239			2 152.611	1.00 18.63	D	C
	MOTA	7010	CG	LEU	239	-1.538	-63.15	3 153.992	1.00 19.49	D	С

-290-

	MOTA	7011	CD1 L	EU	239	-1.136	-64.510	154.487	1.00 16.3	15 I		C
	ATOM	7012	CD2 L	ÆU	239	-1.118	-62.049	154.954	1.00 16.			C
	MOTA	7013		EU	239	-1.012	-63.697	150.268	1.00 20.3	21 1		C
	ATOM	7014	0 I	EU	239			149.819	1.00 19.3	21 I	D	0
5	ATOM	7015		SLU	240	-0.370	-62.755	149.578	1.00 20.			N
	MOTA	7016	CA G	SLU	240		-62.413		1.00 22.	99 1		С
	ATOM	7017		SLU	240	0.069	-61.255	147.664	1.00 25.	70 I		C
	MOTA	7018	CG C	SLU	240	-0.191	-59.897	148.330	1.00 28.	57		C
	ATOM	7019	CD G	SLU	240	-1.584	-59.334	148.036	1.00 32.	06 1	D	C
10	MOTA	7020	OE1 G	SLU	240	-2.437	-60.068	147.492	1.00 33.	41 1	D	0
	MOTA	7021	OE2	3LU	240	-1.834	-58.151	148.358	1.00 34.	50	D	0
	ATOM	7022	C C	GLU	240	-0.649	-63.633	147.304	1.00 22.	86	D	С
	MOTA	7023	0 (GLU	240	-1.510	-63.874	146.469	1.00 22.	97	D	0
	ATOM	7024	N I	LEU	241	0.424	-64.400	147.462	1.00 22.	57	D	N
15	MOTA	7025	CA I	LEU	241	0.618	-65.603	146.655	1.00 23.	67	D	С
	ATOM	7026	CB I	LEU	241	1.948	-66.270	147.035	1.00 25.	60	D	С
	ATOM	7027	CG 1	LEU	241	2.655	-67.315	146.151	1.00 28.		D	С
	ATOM	7028	CD1	LEU	241	1.856	-68.588	146.108	1.00 30.	65	D	С
	MOTA	7029	CD2	LEU	241	2.858	-66.775	144.748	1.00 29.	93	D	С
20	ATOM	7030	C I	LEU	241	-0.567	-66.551	146.931	1.00 22.		D	С
	ATOM	7031		LEU	241			146.013	1.00 21.		D	0
	MOTA	7032		LEU	242			148.201	1.00 21.		D	N
	ATOM	7033		LEU	242			148.588	1.00 20.		D	C
	MOTA	7034		LEU	242			150.114	1.00 21.		D	С
25	ATOM	7035	CG	LEU	242			150.701	1.00 22.	85	D	C
	MOTA	7036	CD1	LEU	242	-3.410	-69.821	150.090	1.00 22.		D	C
	MOTA	7037	CD2	LEU	242			152.211	1.00 22.		D	C
	MOTA	7038		LEU	242			148.017	1.00 20.		D	C
	ATOM	7039		LEU	242			147.438	1.00 19.		D	Ō
30	MOTA	7040		PHE	243			148.160	1.00 19.		D	N
	ATOM	7041		PHE	243			147.646	1.00 19.		D	С
	ATOM	7042	-	PHE	243			148.242	1.00 17.		D	Č
	ATOM	7043		PHE	243			149.650	1.00 16		D	C
	ATOM	7044		PHE	243			150.713	1.00 15		D	Ċ
35	ATOM	7045	CD2		243			149.905	1.00 16.		D	C
	ATOM	7046	_	PHE	243			152.009	1.00 15		D	Ċ
	ATOM	7047	CE2		243			151.204	1.00 16		D	C
	ATOM	7048		PHE	243			152.254	1.00 15		D	C
	ATOM	7049		PHE	243			146.117	1.00 19	.44	D	C
40	ATOM	7050		PHE	243			145.533	1.00 18		D	0
	ATOM	7051		HIS	244			145.474	1.00 19		D	N
	ATOM	7052		HIS	244	-3.804	-65.152	144.016	1.00 20		D	С
	ATOM	7053		HIS	244			143.505	1.00 22		D	C
	ATOM	7054		HIS	244			142.025	1.00 26		D	C
45	MOTA	7055	CD2		244			3 140.999	1.00 27		D	C
	ATOM	7056	ND1		244			141.448	1.00 27		D	N
	ATOM	7057	CE1		244			5 140.134	1.00 27		D	C
	ATOM	7058			244			3 139.836	1.00 27		D	N
	ATOM	7059	С	HIS	244			143.591	1.00 19		D	С
50	ATOM	7060		HIS	244			5 142.621	1.00 18		D	ō
	ATOM	7061	N	PHE	245			144.326	1.00 18		D	N
	ATOM	7062		PHE	245			6 144.036	1.00 17		D	C
	ATOM	7063		PHE	245			1 145.055	1.00 17		D	Ċ
	MOTA	7064		PHE	245			5 145.069	1.00 16		D	Č
55	ATOM	7065			245			7 144.105	1.00 16		D	c
	ATOM	7066			245			4 146.007	1.00 16		D	C
	MOTA	7067		PHE	245			7 144.068			D	C
	ATOM	7068		PHE	245			4 145.984			D	c
	AION	,000	عندت		~ ~ ~	3.372	- ,2.00		2.50 20		_	_

-291-

	3.000	7069	CZ	DUD	245	4 000	72 010	145 000	1 00 15 00	_	^
	MOTA			PHE			-73.812 -69.170		1.00 15.98	D	C
	MOTA	7070 7071	C	PHE	245				1.00 17.44	D	
	ATOM		0	PHE	245		-69.787		1.00 17.41	D	0
5	ATOM	7072		HIS	246		-68.669		1.00 16.27	D	N
3	MOTA	7073		HIS	246		-68.853		1.00 16.76	D	C
	MOTA	7074	CB	HIS	246		-68.409		1.00 14.87	D	C
	MOTA	7075	CG	HIS	246		-69.466		1.00 15.84	D	C
	MOTA	7076	CD2		246		-69.620		1.00 14.94	D	C
40	MOTA	7077	ND1		246		-70.574		1.00 13.95	D	N
10	MOTA	7078	CE1		246			148.816	1.00 14.24	D	C
	MOTA	7079	NE2		246			149.342	1.00 15.38	D	N
	MOTA	7080	C	HIS	246			144.242	1.00 16.72	D	C
	MOTA	7081	0	HIS	246			143.694	1.00 16.62	D	0
	MOTA	7082	N	GLY	247			143.940	1.00 16.82	D	N
15	MOTA	7083	CA	GLY	247			142.907	1.00 18.06	D	C
	MOTA	7084	С	GLY	247			141.569	1.00 18.01	D	C
	MOTA	7085	0	GLY	247			140.867	1.00 18.60	D	0
	MOTA	7086	N	THR	248			141.222	1.00 18.13	D	N
	MOTA	7087	CA	THR	248			139.953	1.00 18.70	D	C
20	MOTA	7088	CB	THR	248			139.763	1.00 18.46	D	C
	MOTA	7089	OG1		248			139.926	1.00 19.05	D	0
	MOTA	7090		THR	248			138.368	1.00 18.69	D	C
	MOTA	7091	С	THR	248			139.878	1.00 18.91	D	C
	MOTA	7092	0	THR	248			138.872	1.00 18.39	D	0
25	MOTA	7093	N	LEU	249			140.943	1.00 19.20	D	N
	MOTA	7094	CA	LEU	249			140.969	1.00 20.23	D	C
	MOTA	7095	CB	LEU	249			142.259	1.00 19.48	D	C
	MOTA	7096	CG	LEU	249			142.443	1.00 20.29	D	C
	MOTA	7097		LEU	249			141.232	1.00 20.40	D	C
30	MOTA	7098		LEU	249			143.713	1.00 18.44	D	C
	MOTA	7099	С	LEU	249			140.867	1.00 20.65	D	С
	MOTA	7100	0	LEU	249			140.109	1.00 19.63	D	0
	MOTA	7101	Ŋ	ARG	250			141.621	1.00 21.15	D	N
	MOTA	7102	CA	ARG	250			141.626	1.00 23.18	D	C
35	MOTA	7103	CB	ARG	250			142.662	1.00 24.41	D	C
	MOTA	7104	CG	ARG	250			143.835	1.00 27.96	D	C
	MOTA	7105	CD	ARG	250			143.403	1.00 27.83	D	C
	MOTA	7106	NE	ARG	250			144.495	1.00 29.89	D	N
4.0	ATOM	7107	CZ	ARG	250			144.354	1.00 32.93	D	С
40	MOTA	7108		ARG	250			145.412	1.00 35.07	D	N
	MOTA	7109		ARG	250			143.159	1.00 33.97	D	N
	ATOM	7110	C	ARG	250			140.284	1.00 23.27	D	C
	MOTA	7111	0	ARG	250			139.972	1.00 21.85	D	0
	ATOM	7112	N	LYS	251			139.504	1.00 24.10	D	N
45	MOTA	7113	CA	LYS	251			138.211	1.00 25.70	D	C
	MOTA	7114	CB	LYS	251			137.640	1.00 26.54	D	C
	ATOM	7115	CG	LYS	251			138.421	1.00 27.85	D	С
	MOTA	7116	CD	LYS	251			2 137.821	1.00 30.19	D	С
	MOTA	7117	CE	LYS	251			138.716	1.00 31.63	D	С
50	MOTA	7118	NZ	LYS	251			5 138.208	1.00 34.50	D	N
	ATOM	7119	С	LYS	251			7 137.190	1.00 26.18	D	C
	MOTA	7120	0	LYS	251			2 136.192	1.00 26.51	D	
	MOTA	7121	N	LEU	252			L 137.431	1.00 26.18	D	
	MOTA	7122	CA	LEU	252			3 136.509	1.00 26.53	D	
55	MOTA	7123	CB	LEU	252			7 136.745	1.00 24.32	D	
	ATOM	7124	CG	LEU	252			7 136.495		D	С
	ATOM	7125		LEU	252			136.786		D	_
	MOTA	7126	CD2	FER TER	252	-9.378	-71.68	1 135.054	1.00 22.08	D	С

	MOTA	7127	С	LEU	252	-13.446	-72.259	136.628	1.00 27.56	D	С
	MOTA	7128	0	LEU	252	-13.794	-73.108	135.812	1.00 28.31	D	0
	ATOM	7129	N	GLN	253	-14.222	-71.868	137.636	1.00 28.57	D	N
	ATOM	7130	CA	GLN	253	-15.556	-72.421	137.863	1.00 29.80	D	С
5	ATOM	7131	CB	GLN	253	-16.554	-71.824	136.862	1.00 31.77	D	C
	ATOM	7132	CG	GLN	253	-16.555	-70.298	136.817	1.00 35.28	D	С
	ATOM	7133	CD	GLN	253	-17.738	-69.711	136.048	1.00 38.18	D	С
	ATOM	7134	OE1	GLN	253	-17.657	-68.597	135.524	1.00 39.03	D	0
	ATOM	7135	NE2	GLN	253	-18.847	-70.451		1.00 39.86	D	N
10	ATOM	7136	С	GLN	253	-15.576	-73.942		1.00 29.42	D	С
	MOTA	7137	0	GLN	253		-74.502		1.00 29.12	D	Ō
	ATOM	7138	N	LEU	254		-74.609		1.00 28.93	D	N
	ATOM	7139	CA	LEU	254		-76.065		1.00 28.81	D	C
	ATOM	7140	СВ	LEU	254		-76.572		1.00 26.92	D	Č
15	ATOM	7141	CG	LEU	254		-76.144		1.00 26.12	D	C
	ATOM	7142		LEU	254		-76.798		1.00 23.47	D	C
	ATOM	7143		LEU	254			137.571	1.00 25.72	D	C
	ATOM	7144	С	LEU	254			139.118	1.00 29.64	D	C
	ATOM	7145	0	LEU	254			139.891	1.00 29.37	D	Ŏ
20	ATOM	7146	N	GLN	255			138.710	1.00 30.18	D	N
	ATOM	7147	CA	GLN	255			139.164	1.00 31.73	D	c
	ATOM	7148	CB	GLN	255			138.003	1.00 34.30	D	c
	ATOM	7149	CG	GLN	255			136.643	1.00 38.01	D	C
	MOTA	7150	CD	GLN	255			135.602	1.00 40.76	D	Ċ
25	ATOM	7151		GLN	255			135.511	1.00 42.15	D	ō
	ATOM	7152	NE2		255			134.789	1.00 42.18	D	N
	MOTA	7153	С	GLN	255			140.251	1.00 31.09	D	C
	ATOM	7154	0	GLN	255			140.292	1.00 29.84	D	0
	ATOM	7155	N	GLU	256			141.127	1.00 30.54	D	N
30	ATOM	7156	CA	GLU	256			142.219	1.00 30.46	D	С
	ATOM	7157	CB	GLU	256			142.920	1.00 32.16	D	C
	ATOM	7158	CG	GLU	256			143.620	1.00 34.89	D	C
	ATOM	7159	CD	GLU	256	-20.223	-81.178	144.663	1.00 35.98	D	С
	MOTA	7160	OE1	GLU	256			144.320	1.00 36.28	D	0
35	ATOM	7161	OE2	GLU	256	-20.194	-80.707	145.820	1.00 36.73	D	0
	MOTA	7162	C	GLU	256	-16.270	-82.041	141.861	1.00 29.44	D	С
	ATOM	7163	0	GLU	256	-15.216	-82.139	142.486	1.00 29.52	D	0
	MOTA	7164	N	PRO	257	-16.578	-82.882	140.862	1.00 28.35	D	N
	MOTA	7165	CD	PRO	257	-17.795	-83.008	140.045	1.00 29.24	D	С
40	ATOM	7166	CA	PRO	257	-15.605	-83.927	140.526	1.00 27.52	D	С
	MOTA	7167	CB	PRO	257	-16.260	-84.659	139.347	1.00 27.78	D	С
	MOTA	7168	CG	PRO	257	-17.266	-83.672	138.815	1.00 29.42	D	С
	ATOM	7169	C	PRO	257	-14.197	-83.416	140.215	1.00 25.67	D	C
	ATOM	7170	0	PRO	257			140.539	1.00 24.99	D	0
45	ATOM	7171	N	GLU	258			139.590	1.00 24.23	D	N
	MOTA	7172	CA	GLU	258	-12.795	-81.671	. 139.273	1.00 22.93	D	C
	MOTA	7173	CB	GLU	258			138.329	1.00 21.97	D	C
	MOTA	7174	CG	GLU	258			136.971	1.00 23.09	D	C
	MOTA	7175	CD	GLU	258			136.109	1.00 22.64	D	С
50	MOTA	7176	OE1	L GLU	258			3 136.653	1.00 22.76	D	0
	MOTA	7177	OE2		258			134.876	1.00 22.39	D	0
	MOTA	7178	С	GLU	258			140.568	1.00 22.29	D	C
	MOTA	7179	О	GLU	258			9 140.733	1.00 21.58	D	0
	MOTA	7180	N	TYR	259			141.484		D	N
55	MOTA	7181	CA	TYR	259			142.762		D	С
	MOTA	7182	CB	TYR	259			143.635		D	С
	ATOM	7183	CG	TYR				5 143.490		D	C
	MOTA	7184	CD:	l TYR	259	-12.170	-77.210	143.825	1.00 18.03	D	С

-293-

	ATOM	7185	CE1		259	-12.205	-75.819	143.728	1.00 16.82	D	C
	ATOM	7186	CD2	TYR	259	-14.429	-77.334	143.047	1.00 17.04	D	C
	ATOM	7187	CE2	TYR	259	-14.478	-75.954	142.940	1.00 16.86	D	C
	ATOM	7188	CZ	TYR	259	-13.363	-75.200	143.285	1.00 17.78	D	С
5	ATOM	7189	ОН	TYR	259	-13.426	-73.832	143.199	1.00 16.55	D	0
	ATOM	7190	C	TYR	259	-11.740			1.00 20.57	D	C
	ATOM	7191	Ö	TYR	259	-10.625			1.00 19.89	D	0
	ATOM	7192	N	VAL	260	-12.568			1.00 20.84	D	N
	ATOM	7193	CA	VAL	260	-12.169			1.00 21.82	D	C
10	ATOM	7194	CB	VAL	260	-13.386			1.00 23.38	D	C
10	ATOM		-		260			143.328	1.00 23.38		c
		7195		VAL						D	
	ATOM	7196		VAL	260			145.719	1.00 24.50	D	С
	ATOM	7197	C	VAL	260	-11.004		143.679	1.00 21.20	D	C
46	MOTA	7198	0	VAL	260		-84.937		1.00 21.64	D	0
15	MOTA	7199	N	LEU	261			142.353	1.00 20.69	D	N
	MOTA	7200	CA	LEU	261			141.656	1.00 21.07	D	С
	MOTA	7201	CB	LEU	261	-10.132	-85.156	140.158	1.00 21.76	D	C
	ATOM	7202	CG	LEU	261	-11.172	-86.227	139.803	1.00 21.71	D	C
	MOTA	7203	CD1	LEU	261	-11.584	-86.102	138.346	1.00 21.95	D	C
20	MOTA	7204	CD2	LEU	261	-10.584	-87.611	140.090	1.00 20.53	D	C
	MOTA	7205	C	LEU	261	-8.553	-84.280	141.897	1.00 21.22	D	С
	MOTA	7206	0	LEU	261			141.996	1.00 21.66	D	0
	ATOM	7207	N	LEU	262			141.999	1.00 21.22	D	N
	ATOM	7208	CA	LEU	262			142.266	1.00 21.43	D	C
25	ATOM	7209	СВ	LEU	262			142.212	1.00 23.16	D	č
	ATOM	7210	CG	LEU	262			141.743	1.00 25.15	D	c
	ATOM	7211		LEU	262			140.390	1.00 23.13	D	C
		7211		LEU	262			141.647	1.00 24.87		c
	ATOM									D	C
30	ATOM	7213	C	LEU	262			143.663	1.00 21.12	D	
30	MOTA	7214	0	LEU	262			143.877	1.00 20.89	D	0
	MOTA	7215	N	ALA	263			144.608	1.00 19.39	D	N
	MOTA	7216	CA	ALA	263			145.972	1.00 19.66	D	C
	MOTA	7217	CB	ALA	263			146.865	1.00 18.64	D	C
	MOTA	7218	C	ALA	263			145.989	1.00 19.63	D	C
35	MOTA	7219	0	ALA	263			146.686	1.00 19.49	D	0
	MOTA	7220	N	ALA	264			145.216	1.00 19.23	D	N
	ATOM	7221	CA	ALA	264	-6.773	-86.639	145.136	1.00 19.14	D	C
	MOTA	7222	CB	ALA	264	-7.670	-87.563	144.300	1.00 18.99	D	С
	MOTA	7223	С	ALA	264	-5.366	-86.566	144.518	1.00 19.43	D	С
40	ATOM	7224	0	ALA	264	-4.451	-87.281	144.940	1.00 18.52	D	0
	ATOM	7225	N	MET	265	-5.193	-85.707	143.517	1.00 18.79	D	N
	MOTA	7226	CA	MET	265	-3.890	-85.582	142.881	1.00 20.11	D	С
	MOTA	7227	СВ	MET	265	-3.980	-84.685	141.642	1.00 21.94	D	С
	ATOM	7228	CG	MET	265			140.467	1.00 23.98	D	C
45	ATOM	7229	SD	MET	265			139.013	1.00 27.16	D	s
	ATOM	7230	CE	MET	265			138.431	1.00 25.04	D	č
	ATOM	7231	C	MET	265			143.868	1.00 19.34	D	C
	ATOM	7232	Ö	MET	265			143.850	1.00 18.51	D	o
					266			144.732	1.00 10.31	D	
50	ATOM	7233	N	ALA					1.00 19.42		И
50	MOTA	7234	CA	ALA	266			145.745		D	C
	ATOM	7235	CB	ALA	266			146.444	1.00 19.09	D	C
	ATOM	7236		ALA	266			2 146.762	1.00 20.30	D	C
	MOTA	7237	0	ALA	266			147.200	1.00 19.06	D	0
	MOTA	7238	N	LEU	267			1 147.125			N
55	ATOM	7239		LEU	267			3 148.080		D	С
	MOTA	7240	CB	LEU	267			5 148.225		D	С
	MOTA	7241	CG	LEU	267	-4.784	-87.89	9 149.565			С
	ATOM	7242		L LEU	267			4 149.295		D	

-294-

	MOTA	7243	CD2	LEU	267	-3.568	-88.082	150.449	1.00 22.95	D	С
	MOTA	7244	С	LEU	267	-2.006	-87.564	147.648	1.00 23.83	D	C
	MOTA	7245	0	LEU	267	-1.107	-87.902	148.412	1.00 23.92	D	0
_	MOTA	7246	N	PHE	268		-88.050		1.00 25.59	D	N
5	MOTA	7247	CA	PHE	268		-89.066		1.00 27.95	D	C
	MOTA	7248	CB	PHE	268	-1.936	-90.039	144.988	1.00 26.41	D	C
	MOTA	7249	CG	PHE	268	-3.071	-90.769	145.657	1.00 25.14	D	С
	MOTA	7250	CD1	PHE	268		-90.525		1.00 24.11	D	C
	MOTA	7251	CD2	PHE	268	-2.822	-91.688	146.676	1.00 25.38	D	C
10	MOTA	7252	CE1	PHE	268	-5.438	-91.176	145.916	1.00 23.69	D	C
	ATOM	7253	CE2	PHE	268	-3.874	-92.351	147.318	1.00 23.66	D	C
	ATOM	7254	CZ	PHE	268	-5.180	-92.093	146.938	1.00 23.71	D	C
	MOTA	7255	С	PHE	268	0.072	-88.558	145.222	1.00 30.43	D	С
	ATOM	7256	0	PHE	268	0.322	-88.862	144.057	1.00 30.67	D	0
15	MOTA	7257	N	SER	269			145.948	1.00 33.96	D	N
	MOTA	7258	CA	SER	269	2.129	-87.277	145.422	1.00 37.03	D	C
	MOTA	7259	CB	SER	269	2.419	-85.877	145.973	1.00 37.39	D	С
	MOTA	7260	OG	SER	269			145.463	1.00 38.30	D	0
	MOTA	7261	С	SER	269	3.192	-88.264	145.896	1.00 39.10	D	C
20	MOTA	7262	0	SER	269	3.421	-88.411	147.096	1.00 38.72	D	0
	ATOM	7263	N	PRO	270	3.843	-88.969	144.954	1.00 41.49	D	N
	MOTA	7264	CD	PRO	270	3.602	-88.913	143.499	1.00 41.60	D	C
	ATOM	7265	CA	PRO	270	4.884	-89.957	145.270	1.00 43.13	D	С
	MOTA	7266	CB	PRO	270	5.051	-90.704	143.951	1.00 42.69	D	C
25	MOTA	7267	CG	PRO	270	4.821	-89.621	142.940	1.00 42.36	D	C
	MOTA	7268	С	PRO	270	6.211	-89.397	145.782	1.00 44.56	D	C
	MOTA	7269	0	PRO	270	7.015	-90.131	146.361	1.00 45.15	D	0
	MOTA	7270	N	ASP	271	6.441	-88.105	145.577	1.00 45.55	D	N
	ATOM	7271	CA	ASP	271	7.687	-87.482	146.010	1.00 46.83	D	С
30	ATOM	7272	CB	ASP	271	8.101	-86.413	144.996	1.00 48.20	D	C
	MOTA	7273	CG	ASP	271	7.070	-85.312	144.852	1.00 49.90	D	С
	ATOM	7274	OD1	ASP	271	5.860	-85.620	144.759	1.00 50.47	D	0
	ATOM	7275	OD2	ASP	271	7.475	-84.131	144.818	1.00 50.92	D	0
	ATOM	7276	С	ASP	271	7.636	-86.886	147.418	1.00 47.00	D	C
35	MOTA	7277	0	ASP	271	8.521	-86.124	147.815	1.00 47.50	D	0
	MOTA	7278	N	ARG	272	6.602	-87.243	148.172	1.00 46.37	D	N
	MOTA	7279	CA	ARG	272	6.436	-86.762	149.534	1.00 45.93	D	С
	MOTA	7280	CB	ARG	272			150.050	1.00 45.63	D	C
	MOTA	7281	CG	ARG	272	4.218	-85.980	150.556	1.00 44.83	D	С
40	MOTA	7282	CD	ARG	272		-85.410		1.00 42.90	D	С
	MOTA	7283	NE	ARG	272	3.425	-83.961	L 149.425	1.00 41.67	D	N
	MOTA	7284	CZ	ARG	272			3 148.936		D	С
	ATOM	7285		ARG	272			3 148.445	1.00 38.84	D	N
	MOTA	7286		ARG	272			148.939	1.00 40.16	D	N
45	MOTA	7287	C	ARG	272			5 150.435	1.00 46.08	D	С
	MOTA	7288	0	ARG	272			5 150.246	1.00 45.78	D	0
	MOTA	7289	N	PRO	273			4 151.428	1.00 46.22	D	N
	MOTA	7290	CD	PRO	273			1 151.712	1.00 45.76	D	C
	MOTA	7291		PRO	273			3 152.334	1.00 46.41	D	С
50	MOTA	7292		PRO	273			4 153.132	1.00 46.21	D	C
	MOTA	7293		PRO	273			9 153.133	1.00 46.57	D	C
	MOTA	7294		PRO	273			2 153.233	1.00 46.69	D	С
	MOTA	7295		PRO	273			0 153.938	1.00 46.36	D	
	MOTA	7296		GLY	274			7 153.193	1.00 46.90	D	
55	ATOM	7297		GLY	274			2 154.010		D	
	ATOM	7298	С	GLY	274			6 153.314			_
	MOTA	7299		GLY	274			5 153.951			_
	ATOM	7300	N	VAL	275	7.748	3 -91.46	2 152.012	1.00 48.62	D	N

-295-

	ATOM	7301	CA	VAL	275	6.938 -92.4	411 151.259	1.00 49.05	D	C
	ATOM	7302	CB	VAL	275	6.392 -91.	779 149.953	1.00 48.86	D	C
	ATOM	7303	CG1	VAL	275	5.673 -92.8	B33 149.121	1.00 48.34	D	С
_	ATOM	7304	CG2	VAL	275	5.440 -90.0	640 150.289	1.00 47.97	D	C
5	MOTA	7305	С	VAL	275	7.726 -93.	669 150.913	1.00 49.50	D	C
	MOTA	7306	0	VAL	275	8.835 -93.	599 150.386	1.00 49.51	D	0
	MOTA	7307	N	THR	276		818 151.224	1.00 50.30	D	N
	ATOM	7308	CA	THR	276		112 150.957	1.00 51.08	D	C
	ATOM	7309	СВ	THR	276		168 151.975	1.00 51.15	D	C
10	ATOM	7310		THR	276		838 153.277	1.00 51.62	D	0
	ATOM	7311		THR	276		559 151.590	1.00 51.91	D	Ċ
	ATOM	7312	C	THR	276		590 149.542	1.00 51.59	D	Ċ
	ATOM	7313	ō	THR	276		729 148.710	1.00 52.05	D	ō
	ATOM	7314	N	GLN	277		836 149.278	1.00 51.49	D	N
15	ATOM	7315	CA	GLN	277		304 147.973	1.00 51.75	D	c
	MOTA	7316	СВ	GLN	277		023 148.118	1.00 52.32	D	Č
	ATOM	7317	CG	GLN	277		373 148.796	1.00 53.71	D	Ċ
	ATOM	7318	CD	GLN	277		079 148.880	1.00 54.80	D	Č
	ATOM	7319	OE1		277		020 147.951	1.00 55.58	D	ō
20	ATOM	7320		GLN	277		768 149.988	1.00 55.24	D	N
	ATOM	7321	C	GLN	277		180 146.946	1.00 51.46	D	c
	ATOM	7322	ŏ	GLN	277		884 146.460	1.00 51.02	D	ŏ
	MOTA	7323	N	ARG	278		569 146.615	1.00 51.45	D	N
	ATOM	7324	CA	ARG	278		475 145.654	1.00 51.57	D	Ċ
25	ATOM	7325	СВ	ARG	278		012 145.504	1.00 52.92	D	č
	ATOM	7326	CG	ARG	278		073 144.340	1.00 55.26	D	c
	ATOM	7327	CD	ARG	278		845 143.046	1.00 57.26	D	Č
	ATOM	7328	NE	ARG	278		037 142.049	1.00 58.68	D	N
	ATOM	7329	CZ	ARG	278		627 142.159	1.00 59.43	D	c
30	ATOM	7330		ARG	278		945 143.228	1.00 59.27	D	Ň
	ATOM	7331		ARG	278		892 141.194	1.00 59.72	D	N
	ATOM	7332	С	ARG	278		846 144.296	1.00 50.85	D	c
	ATOM	7333	Ö	ARG	278		059 143.693	1.00 50.65	D	Ō
	ATOM	7334	N	ASP	279		046 143.821	1.00 50.22	D	N
35	ATOM	7335	CA	ASP	279		516 142.532	1.00 49.17	D	С
	ATOM	7336	СВ	ASP	279		818 142.151	1.00 51.29	D	C
	ATOM	7337	CG	ASP	279		.585 141.643	1.00 53.01	D	Ċ
	ATOM	7338		ASP	279		.739 142.221	1.00 54.57	D	Ō
	MOTA	7339		ASP	279		.254 140.667	1.00 54.28	D	0
40	ATOM	7340	C	ASP	279		.718 142.508	1.00 47.62	D	Ċ
	ATOM	7341	ō	ASP	279		.316 141.560	1.00 47.32	D	ō
	ATOM	7342	N	GLU	280		.343 143.548	1.00 46.06	D	N
	MOTA	7343	CA	GLU	280	2.495 -97	.579 143.622	1.00 44.64	D	C
	MOTA	7344		GLU	280		.466 144.826	1.00 45.89	D	C
45	MOTA	7345		GLU	280	2.755 -99	.866 144.754		D	C
	ATOM	7346		GLU	280	4.074 -99	.997 145.509		D	C
	ATOM	7347		GLU	280	4.986 -99	.165 145.302		D	0
	ATOM	7348		GLU	280		.947 146.312		D	0
	ATOM	7349		GLU	280		.260 143.715		D	С
50	ATOM	7350		GLU	280		.074 143.045		Ø	0
	ATOM	7351		ILE	281	2.213 -95	.348 144.550	1.00 41.01	D	N
	ATOM	7352		ILE	281		.053 144.706		D	
	ATOM	7353		ILE	281		.277 145.900		D	
	ATOM	7354		ILE	281		.847 145.919		D	
55	ATOM	7355		ILE	281		.997 147.206		D	
	ATOM	7356		LILE	281		.392 148.443		D	
	ATOM	7357		ILE			.231 143.420		D	
	ATOM	7358		ILE			.466 143.069		D	
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-296-

	MOTA	7359	N	ASP	282	2.810	-93.405	142.718	1.00 39.49	D N	
	ATOM	7360	CA	ASP	282	3.049	-92.698	141.465	1.00 39.92	D C	
	ATOM	7361	CB	ASP	282	4.440	-93.042	140.924	1.00 42.08	D C	
	MOTA	7362	CG	ASP	282	4.997	-91.967	140.010	1.00 44.33	D C	
5	MOTA	7363	OD1	ASP	282	4.385	-91.694	138.956	1.00 45.27	D O	1
	MOTA	7364	OD2	ASP	282	6.053	-91.388	140.351	1.00 46.09	D O	,
	MOTA	7365	С	ASP	282	1.977	-93.115	140.453	1.00 39.04	D C	;
	MOTA	7366	0	ASP	282	1.403	-92.273	139.762	1.00 38.00	D O	,
	ATOM	7367	N	GLN	283		-94.417		1.00 38.52	D N	
10	MOTA	7368	CA	GLN	283	0.691	-94.943	139.471	1.00 38.31	D C	
	ATOM	7369	СВ	GLN	283	0.725	-96.476	139.448	1.00 40.70	D C	
	ATOM	7370	CG	GLN	283			139.041	1.00 44.18	D C	
	ATOM	7371	CD	GLN	283		-	138.677	1.00 46.41	D C	
	ATOM	7372	OE1		283			139.404	1.00 47.67	D C	
15	ATOM	7373	NE2		283			137.546	1.00 46.87	D N	
• •	ATOM	7374	C	GLN	283			139.860	1.00 36.85	D C	
	ATOM	7375	ō	GLN	283			139.000	1.00 36.29	D C	
	ATOM	7376	N	LEU	284			141.159	1.00 35.69	D N	
	ATOM	7377	CA	LEU	284			141.624	1.00 34.25	D C	
20	ATOM	7378	СВ	LEU	284		-	143.153	1.00 33.82	D C	
	ATOM	7379	CG	LEU	284			143.747	1.00 33.47	D C	
	ATOM	7380	-	LEU	284			145.259	1.00 32.83	D	
	ATOM	7381		LEU	284			143.164	1.00 32.79	D C	
	ATOM	7382	c	LEU	284			141.171	1.00 33.26	D C	
25	ATOM	7383	Ö	LEU	284			140.781	1.00 31.51	D	
	ATOM	7384	N	GLN	285			141.216	1.00 33.02	Di	
	ATOM	7385	CA	GLN	285			140.794	1.00 33.96		3
	ATOM	7386	СВ	GLN	285			141.037	1.00 34.10		Ĉ
	ATOM	7387	CG	GLN	285			140.713	1.00 35.79		c
30	ATOM	7388	CD	GLN	285			141.077	1.00 36.64		C
•	ATOM	7389		GLN	285			140.461	1.00 38.71		0
	ATOM	7390	NE2		285			142.095	1.00 36.76		N
	ATOM	7391	C	GLN	285			139.317	1.00 33.52		C
	ATOM	7392	ŏ	GLN	285			138.923	1.00 33.70		ō
35	ATOM	7393	N	GLU	286			138.501	1.00 33.33		N
•	ATOM	7394	CA	GLU	286			137.069	1.00 34.29		C
	ATOM	7395	СВ	GLU	286			136.358	1.00 36.73		Č
	ATOM	7396	CG	GLU	286			136.801	1.00 41.05		C
	ATOM	7397	CD	GLU	286	1.897		135.919	1.00 44.06		c
40	ATOM	7398	OE1		286	1.725		135.629	1.00 46.05		ō
	ATOM	7399		GLU	286			135.525	1.00 45.70		ō
	ATOM	7400	C		286			136.817	1.00 32.71		Č
	ATOM	7401	Ö	GLU	286			5 135.951	1.00 31.80		ō
	ATOM	7402	N	GLU	287			137.593	1.00 32.21		N
45	ATOM	7403	CA	GLU	287			3 137.467	1.00 31.48		C
	ATOM	7404	СВ	GLU	287			138.421	1.00 33.15		c
	ATOM	7405	CG	GLU	287			138.208	1.00 36.26		c
	ATOM	7406	CD	GLU	287			5 139.278	1.00 38.20	D	Č
	ATOM	7407		GLU	287			1 139.634	1.00 38.75	D	ō
50	MOTA	7408		GLU	287			3 139.752	1.00 38.76		ō
-	ATOM	7409		GLU	287			7 137.787	1.00 29.64		č
	ATOM	7410		GLU	287			3 137.122	1.00 30.00		ŏ
	ATOM	7411		MET	288			8 138.818			N
	ATOM	7412		MET	288			9 139.197	1.00 27.18		C
55	MOTA	7413		MET	288			6 140.464			C
	MOTA	7414		MET	288			0 140.404			C
	MOTA	7415		MET	288			1 142.292		D	s
	ATOM	7416		MET	288			4 141.971			C
	AION	,410		PIET	200	-0.043	, - , 2 . 2 0	- 1-1.7/1	1.00 27.72	•	~

-297-

	MOTA	7417	С	MET	288	-6.207	-88.592	138.040	1.00 26.19	D	С
	MOTA	7418	0	MET	288	-7.231	-88.074	137.607	1.00 25.68	D	0
	MOTA	7419	N	ALA	289	-4.999	-88.348	137.539	1.00 25.78	D	N
_	MOTA	7420		ALA	289	-4.771	-87.407	136.440	1.00 25.91	D	C
5	ATOM	7421		ALA	289		-87.358		1.00 24.39	D	C
	MOTA	7422	С	ALA	289	-5.580	-87.746	135.185	1.00 25.97	D	С
	MOTA	7423	0	ALA	289	-6.245	-86.883	134.605	1.00 25.73	D	0
	ATOM	7424	N	LEU	290	-5.526	-89.003	134.765	1.00 26.73	D	N
	ATOM	7425	CA	LEU	290	-6.260	-89.423	133.585	1.00 27.49	D	С
10	ATOM	7426	CB	LEU	290	-5.920	-90.873	133.238	1.00 30.25	D	С
	ATOM	7427	CG	LEU	290	-4.511	-91.055	132.662	1.00 31.14	D	С
	MOTA	7428	CD1	LEU	290	-4.257	-92.519	132.347	1.00 32.31	D	C
	MOTA	7429	CD2	LEU	290	-4.383	-90.217	131.402	1.00 32.28	D	С
	MOTA	7430	С	LEU	290	-7.759	-89.265	133.767	1.00 26.79	D	С
15	ATOM	7431	0	LEU	290	-8.458	-88.847	132.845	1.00 26.47	D	0
	ATOM	7432	N	THR	291	-8.255	-89.596	134.955	1.00 25.93	D	N
	ATOM	7433	CA	THR	291	-9.683	-89.466	135.231	1.00 25.58	D	С
	MOTA	7434	CB	THR	291	-10.017	-89.994	136.638	1.00 25.08	D	C
	MOTA	7435	OG1	THR	291	-9.603	-91.361	136.735	1.00 24.28	D	0
20	MOTA	7436	CG2	THR	291			136.912	1.00 24.63	D	C
	ATOM	7437	C	THR	291			135.112	1.00 25.32	D	C
	ATOM	7438	0	THR	291			134.558	1.00 25.11	D	O
	MOTA	7439	N	LEU	292			135.639	1.00 25.55	D	N
	ATOM	7440	CA	LEU	292			135.559	1.00 26.33	D	C
25	ATOM	7441	СВ	LEU	292			136.344	1.00 25.09	D	C
	ATOM	7442	CG	LEU	292			136.197	1.00 24.67	D	C
	ATOM	7443		LEU	292			136.510	1.00 23.71	D	C
	ATOM	7444		LEU	292			137.130	1.00 23.44	D	Č
	ATOM	7445	C	LEU	292			134.099	1.00 27.35	D	Č
30	ATOM	7446	ō	LEU	292			133.670	1.00 26.47	D	ō
	ATOM	7447	N	GLN	293			133.344	1.00 29.48	D	N
	ATOM	7448	CA	GLN	293			131.928	1.00 32.08	D	C
	ATOM	7449	СВ	GLN	293			131.301	1.00 34.17	D	c
	ATOM	7450	CG	GLN	293			131.910	1.00 37.03	D	Č
35	ATOM	7451	CD	GLN	293			131.347	1.00 39.59	D	C
	ATOM	7452		GLN	293			130.129	1.00 41.51	D	ō
	ATOM	7453	NE2		293			132.232	1.00 40.22	D	N
	ATOM	7454	C	GLN	293			131.198	1.00 32.47	D	C
	ATOM	7455	Ō	GLN	293			130.489	1.00 31.68	D	ō
40	ATOM	7456	N	SER	294			131.386	1.00 33.78	D	N
	ATOM	7457	CA	SER	294			130.760	1.00 35.43	D	C
	MOTA	7458	СВ	SER	294			131.185	1.00 35.97	D	C
	ATOM	7459	OG	SER	294	-10.173	-89.898	130.763	1.00 38.15	D	o
	ATOM	7460	C	SER	294			131.130	1.00 35.91	D	C
45	ATOM	7461	Ō	SER	294			130.282	1.00 36.34	D	o
	ATOM	7462	N	TYR	295			132.400	1.00 35.87	D	N
	ATOM	7463	CA	TYR	295			132.830	1.00 36.69	D	C
	ATOM	7464	СВ	TYR	295			3 134.350	1.00 35.73	D	C
	ATOM	7465		TYR	295			134.855	1.00 34.69	D	C
50	ATOM	7466			295			2 134.827	1.00 34.72	D	C
-	ATOM	7467		TYR	295			3 135.226	1.00 34.93	D	Č
	ATOM	7468			295			3 135.304	1.00 35.18	D	C
	ATOM	7469			295			135.706	1.00 34.88	D	c
	ATOM	7470		TYR	295			7 135.662	1.00 35.17	D	Ċ
55	ATOM	7471		TYR	295			136.034	1.00 35.12	D	Ö
55	ATOM	7472		TYR	295			3 132.119		D	C
	MOTA	7473		TYR	295			5 131.651		D	
	ATOM	7474		ILE	296			3 132.040		D	
	VI ON	/4/4	TA	ئابىي	250	-12.111	-00,010	- 102.UEV	2.00 00.00		TA

-298-

		2426	~		296	-12.745	02 614	121 277	1.00	41 00	D ·	С
	ATOM	7475		ILE ILE	296 296	-11.348			1.00			C
	ATOM	7476							1.00			C
	MOTA	7477		ILE	296			130.637	1.00			C
5	MOTA	7478	CG1		296	-11.105			1.00			C
J	ATOM	7479	CD1		296	-9.736		133.259				C
	MOTA	7480		ILE	296	-13.091			1.00			
	MOTA	7481		ILE	296		-	129.347		42.30		0
	MOTA	7482		LYS	297		-83.673			45.50		N
40	MOTA	7483		LYS	297	-12.792				48.44	D	C
10	MOTA	7484		LYS	297	-11.960				48.12	D	C
	MOTA	7485		LYS	297		-84.861			48.26	D	C
	MOTA	7486		LYS	297		-86.096			49.23	D	C
	MOTA	7487		LYS	297		-85.891			50.24	D	С
46	MOTA	7488		LYS	297		-87.102			50.73	D	N
15	MOTA	7489		LYS	297		-84.245			50.60	D	C
	MOTA	7490	0	LYS	297		-83.690			50.62	D	0
	MOTA	7491	N	GLY	298		-85.151			53.71	D	N
	MOTA	7492	CA	GLY	298		-85.527			57.58	D	C
00	MOTA	7493	С	GLY	298		-84.372			60.34	D	C
20	ATOM	7494	0	GLY	298		-83.664			60.81	D	0
	MOTA	7495	N	GLN	299		-84.180			63.65	D	N
	MOTA	7496	CA	GLN	299		-83.108			66.89	D	С
	MOTA	7497	CB	GLN	299		-83.099			67.10	D	C
05	MOTA	7498	CG	GLN	299		-82.244			68.11	D	C
25	MOTA	7499	CD	GLN	299		-80.773			68.71	D	C
	MOTA	7500		GLN	299		-80.153			69.05	D	0
	MOTA	7501	NE2	GLN	299		-80.205			69.38	D	N
	ATOM	7502	С	GLN	299		-81.745			68.91	D	C
20	MOTA	7503	0	GLN	299		-81.171			69.02	D	0
30	MOTA	7504	N	GLN	300		-81.239			71.20	D	N
	MOTA	7505	CA	GLN	300		-79.938			73.67	D	C
	MOTA	7506	CB	GLN	300		-79.872			74.21	D	C
	MOTA	7507	CG	GLN	300		-81.023			75.16	D	C
35	ATOM	7508	CD	GLN	300		-80.605			75.58	D	
33	ATOM	7509	OE1		300		-80.174			75.70	D	N O
	ATOM	7510		GLN	300		-80.726			75.83	D	C
	ATOM	7511	C	GLN	300		-79.598			74.94 75.30	D D	0
	ATOM	7512	0	GLN	300			127.454 125.972		76.23	D	И
40	ATOM	7513	N	ARG	301			123.372		77.42	D	C
70	ATOM	7514	CA	ARG	301			124.773		77.89	D	C
	ATOM	7515	CB	ARG	301 301			123.354		78.74	D	C
	MOTA MOTA	7516 7517	CD	ARG ARG	301			122.388		79.60	D	c
	ATOM	7518		ARG	301			122.053		79.99	Ď	N
45	ATOM	7519		ARG	301			121.181		80.24	D	C
.0	ATOM	7520		ARG	301			120.529		80.26	D	N
	ATOM	7521		ARG	301			120.969		80.28	D	N
	ATOM	7521		ARG	301			124.705		77.75	D	c
	ATOM	7523		ARG	301			123.624		78.10	D	ŏ
50	ATOM	7524		ARG	302			125.868		77.90	D	N
-	MOTA	7525		ARG	302			125.980		77.67	D	C
	MOTA	7525 7526		ARG	302			126.965		78.48	D	Č
	ATOM	7527		ARG	302			126.880		79.56	D	Č
	ATOM	7528		ARG	302			125.564		80.20	D	Č
55	ATOM	7529		ARG	302			125.360		81.19	D	N
	ATOM	7530		ARG	302			124.499		81.77	D	c
	ATOM	7531		L ARG	302			123.749		81.87		Ň
	ATOM	7532		2 ARG	302			124.386		81.98		
	AT ON	1332	. TAIT		302	,,			,		_	

-299-

	ATOM	7533	С	ARG	302	-18.911	-75.032	126.498	1.00 76.83	D	C
	MOTA	7534	0	ARG	302	-18.303	-74.206	125.812	1.00 77.05	D	0
	MOTA	7535	N	PRO	303	-18.459	-75.423	127.711	1.00 75.72	D	N
	MOTA	7536	CD	PRO	303	-18.978	-76.402	128.687	1.00 75.41	D	C
5	MOTA	7537	CA	PRO	303	-17.215	-74.820	128.201	1.00 74.46	D	C
	MOTA	7538	CB	PRO	303	-16.951	-75.576	129.505	1.00 74.67	D	C
	MOTA	7539	CG	PRO	303	-18.322	-75.955	129.968	1.00 75.17	D	C
	MOTA	7540	С	PRO	303	-16.100	-75.043	127.180	1.00 73.06	D	C
	ATOM	7541	0	PRO	303	-15.406	-74.104	126.783	1.00 73.11	D	0
10	ATOM	7542	N	ARG	304	-15.962	-76.298	126.753	1.00 71.01	D	N
	ATOM	7543	CA	ARG	304	-14.947	-76.711	125.791	1.00 68.70	D	C
	MOTA	7544	CB	ARG	304	-15.518	-76.711	124.369	1.00 69.88	D	С
	ATOM	7545	CG	ARG	304	-14.832	-77.704	123.428	1.00 71.21	D	C
	ATOM	7546	CD	ARG	304	-13.434	-77.252	123.009	1.00 72.37	D	С
15	ATOM	7547	NE	ARG	304	-12.645	-78.321	122.386	1.00 73.31	D	N
-	ATOM	7548	CZ	ARG	304			121.254	1.00 73.71	D	С
•	ATOM	7549	-	ARG	304			120.578	1.00 74.08	D	N
	ATOM	7550		ARG	304			120.792	1.00 73.93	D	N
	ATOM	7551	С	ARG	304			125.869	1.00 66.18	D	C
20	ATOM	7552	ō	ARG	304			125.054	1.00 66.00	D	O
	ATOM	7553	N	ASP	305			126.884	1.00 63.00	D	N
	ATOM	7554	CA	ASP	305			127.091	1.00 59.34	D	C
	MOTA	7555	CB	ASP	305			128.414	1.00 59.31	D	Č
	ATOM	7556	CG	ASP	305			128.703	1.00 59.38	D	č
25	MOTA	7557		ASP	305			127.766	1.00 59.54	D	ō
	MOTA	7558	OD2		305			129.861	1.00 59.45	D	ŏ
	ATOM	7559	C	ASP	305			127.100	1.00 56.66	D	c
	ATOM	7560	0	ASP	305			128.036	1.00 56.22	D	ō
	ATOM	7561	Ŋ	ARG	306			126.042	1.00 52.93	D	N
30	ATOM	7562	CA	ARG	306			125.926	1.00 49.32	D	c
00	ATOM	7563	CB	ARG	306			124.487	1.00 50.93	D	C
	ATOM	7564	CG	ARG	306			123.481	1.00 52.84	D	c
	ATOM	7565	CD	ARG	306			122.147	1.00 54.60	D	Č
	ATOM	7566	NE	ARG	306			121.500	1.00 56.43	D	N
35	ATOM	7567	CZ	ARG	306			120.917	1.00 57.34	D	C
00	MOTA	7568	NH1		306			120.887	1.00 58.29	D	N
	ATOM	7569	NH2		306			120.367	1.00 57.94	D	N
	MOTA	7570	C	ARG	306			126.879	1.00 45.59	D	C
	ATOM	7571	Ö	ARG	306			127.086	1.00 45.21	D	ō
40	ATOM	7572	N	PHE	307			3 127.456	1.00 41.34	D	N
40	ATOM	7573	CA	PHE	307			128.378	1.00 37.64	D	C
	ATOM	7574	CB	PHE	307			l 128.244	1.00 37.62	D	
	ATOM	7575	CG	PHE	307			3 126.876	1.00 37.02	D	C
		7576		PHE	307			5 125.872	1.00 38.94	D	C
45	MOTA				307			126.580	1.00 38.30	D	c
70	ATOM	7577		PHE	307			3 124.591	1.00 38.89	D	c
	MOTA	7578		PHE				9 125.305	1.00 38.37	D	C
	ATOM	7579		PHE	307			1 124.309	1.00 38.57	D	C
	ATOM	7580		PHE	307			2 129.855	1.00 34.77	D	C
50	MOTA	7581		PHE	307			9 130.692	1.00 34.77		
30	ATOM	7582		PHE	307						
	ATOM	7583		LEU	308			3 130.174 6 131 559			
	ATOM	7584		LEU	308			6 131.558			
	ATOM	7585		LEU	308			5 131.625			
65	ATOM	7586		LEU	308			7 132.793			
55	ATOM	7587		1 LEU	308			1 132.946			
	MOTA	7588		2 LEU	308			8 134.081			
	ATOM	7589		LEU	308			2 132.311			_
	ATOM	7590	0	LEU	308	-6.72	4 -76.79	7 133.345	1.00 24.44	D	0

-300-

	MOTA	7591	N	TYR	309	-7.079	-78.385	131.810	1.00 24.84	D	N
	MOTA	7592	CA	TYR	309	-6.199	-79.333	132.489	1.00 24.89	D	С
	MOTA	7593	CB	TYR	309	-6.107	-80.634	131.691	1.00 24.35	D	C
_	MOTA	7594	CG	TYR	309		-81.708		1.00 25.38	D	C
5	MOTA	7595	CD1		309		-82.214		1.00 24.51	D	С
	MOTA	7596	CE1	TYR	309		-83.203		1.00 24.34	D	C
	MOTA	7597	CD2	TYR	309		-82.220		1.00 24.33	D	C
	ATOM	7598	CE2	TYR	309	-3.372	-83.215	132.410	1.00 24.59	D	С
	ATOM	7599	CZ	TYR	309	-3.781	-83.698	133.650	1.00 24.77	D	C
10	ATOM	7600	OH	TYR	309	-3.061	-84.683	134.288	1.00 25.73	D	0
	ATOM	7601	С	TYR	309	-4.794	-78.774	132.732	1.00 24.60	D	C
	MOTA	7602	0	TYR	309		-78.888		1.00 24.29	D	0
	MOTA	7603	N	ALA	310		-78.171		1.00 23.83	D	N
	MOTA	7604	CA	ALA	310		-77.601		1.00 23.53	D	C
15	MOTA	7605	CB	ALA	310	-2.445	-76.970	130.498	1.00 22.84	D	C
	MOTA	7606	C	ALA	310	-2.843	-76.562	132.948	1.00 22.76	D	C
	MOTA	7607	0	ALA	310		-76.522		1.00 21.87	D	0
	MOTA	7608	N	LYS	311	-3.868	-75.715	133.010	1.00 22.43	D	N
	MOTA	7609	CA	LYS	311	-3.943	-74.707	134.063	1.00 22.75	D	C
20	MOTA	7610	СВ	LYS	311	-5.146	-73.782	133.858	1.00 23.52	D	C
	MOTA	7611	CG	LYS	311	-4.926	-72.669	132.843	1.00 25.26	D	С
	MOTA	7612	CD	LYS	311	-6.227	-71.915	132.590	1.00 27.42	D	C
	MOTA	7613	CE	LYS	311	-6.022	-70.752	131.630	1.00 30.14	D	C
	MOTA	7614	NZ	LYS	311	-7.321	-70.118	131.265	1.00 32.77	D	N
25	MOTA	7615	C	LYS	311	-4.039	-75.359	135.444	1.00 22.13	D	С
	MOTA	7616	0	LYS	311	-3.433	-74.877	136.399	1.00 21.60	D	0
	MOTA	7617	N	LEU	312			135.547	1.00 20.89	D	N
	MOTA	7618	CA	LEU	312	-4.950	-77.139	136.823	1.00 21.30	D	С
	MOTA	7619	CB	LEU	312	-6.033	~78.219	136.726	1.00 20.26	D	С
30	MOTA	7620	CG	LEU	312	-7.442	-77.639	136.538	1.00 20.91	D	С
	MOTA	7621	CD1	LEU	312	-8.472	-78.737	136.375	1.00 19.59	D	С
	MOTA	7622	CD2	LEU	312	-7.775	-76.766	137.740	1.00 21.76	D	С
	MOTA	7623	С	LEU	312	-3.624	-77.737	137.292	1.00 21.85	D	С
	ATOM	7624	0	LEU	312			138.483	1.00 20.99	D	0
35	MOTA	7625	N	LEU	313			136.365	1.00 20.96	D	N
	MOTA	7626	CA	LEU	313	-1.539	-78.833	136.736	1.00 21.57	D	C
	ATOM	7627	CB	LEU	313			135.541	1.00 20.84	D	C
	MOTA	7628	CG	LEU	313			135.048	1.00 21.35	D	C
4.0	MOTA	7629		LEU	313			134.016	1.00 19.73	D	С
40	MOTA	7630		LEU	313			136.234	1.00 21.46	D	C
	MOTA	7631	С	LEU	313	-0.668	-77.683	137.230	1.00 21.97	D	С
	MOTA	7632	0	LEU	313			138.190	1.00 21.62	D	O
	MOTA	7633	N	GLY	314			136.573	1.00 22.24	D	N
45	ATOM	7634	CA	GLY	314			136.980	1.00 22.60	D	C
45	MOTA	7635	C	GLY	314			138.383	1.00 23.14	D	С
	MOTA	7636	0	GLY	314			139.198	1.00 22.01	D	0
	MOTA	7637	N	LEU	315			138.667	1.00 23.45	D	N
	MOTA	7638	CA	LEU	315			139.986	1.00 24.19	D	С
50	MOTA	7639	CB	LEU	315			139.979	1.00 24.08	D	C
50	MOTA	7640	CG	LEU	315			139.404	1.00 25.31	D	C
	MOTA	7641		LEU	315			139.159	1.00 24.47	D	С
	MOTA	7642		LEU	315			140.383	1.00 24.52	D	C
	MOTA	7643	С	LEU	315			141.055	1.00 23.53	D	C
	MOTA	7644		LEU	315			142.213	1.00 23.85	D	0
55	MOTA	7645		LEU	316			140.667	1.00 23.29	D	N
	MOTA	7646		LEU	316			141.605	1.00 23.36	D	С
	ATOM	7647		LEU	316			140.982	1.00 24.00	D	С
	MOTA	7648	CG	LEU	316	-2.589	-79.846	141.012	1.00 26.29	D	С

-301-

	ATOM	7649	CD1		316		-81.247		1.00 25.87	D	C
	MOTA	7650	CD2		316	-3.090	-79.904	142.453	1.00 25.54	D	C
	MOTA	7651	С	LEU	316	0.346	-77.572	142.028	1.00 22.98	D	C
_	ATOM	7652	0	LEU	316	0.704	-77.776	143.189	1.00 22.32	D	0
5	MOTA	7653	N	ALA	317		-77.134		1.00 22.45	D	N
	MOTA	7654	CA	ALA	317	2.567	-76.815	141.374	1.00 22.43	D	С
	MOTA	7655	CB	ALA	317	3.355	-76.602	140.072	1.00 21.73	D	C
	MOTA	7656	C	ALA	317	2.599	-75.543	142.236	1.00 22.46	D	C
40	ATOM	7657	0	ALA	317		-75.435		1.00 21.94	D	0
10	ATOM	7658	N	GLU	318	1.736	-74.581	141.923	1.00 22.48	D	N
	ATOM	7659	CA	GLU	318	1.681	-73.353	142.706	1.00 23.87	D	C
	MOTA	7660	CB	GLU	318	0.666	-72.364	142.122	1.00 25.70	D	C
	MOTA	7661	CG	GLU	318	0.508	-71.114	142.984	1.00 31.16	D	С
45	MOTA	7662	CD	GLU	318	-0.110	-69.941	142.249	1.00 34.23	D	C
15	ATOM	7663	OE1	GLU	318	-1.252	-70.057	141.761	1.00 36.85	D	0
	ATOM	7664	OE2	GLU	318	0.553	-68.888	142.164	1.00 37.30	D	0
	ATOM	7665	С	GLU	318	1.297	-73.687	144.144	1.00 23.13	D	C
	MOTA	7666	0	GLU	318	1.880	-73.163	145.095	1.00 21.66	D	0
	MOTA	7667	N	LEU	319	0.314	-74.569	144.299	1.00 22.62	D	N
20	MOTA	7668	CA	LEU	319	-0.130	-74.982	145.623	1.00 22.59	D	C
	ATOM	7669	CB	LEU	319	-1.309	-75.953	145.491	1.00 22.32	D	C
	ATOM	7670	CG	LEU	319	-2.055	-76.411	146.743	1.00 22.65	D	C
	ATOM	7671	CD1	LEU	319	-2.451	-75.211	147.601	1.00 19.98	D	C
	ATOM	7672	CD2	LEU	319	-3.290	-77.207	146.314	1.00 21.48	D	С
25	MOTA	7673	C	LEU	319	1.046	-75.647	146.349	1.00 22.54	D	С
	MOTA	7674	0	LEU	319	1.216	-75.492	147.560	1.00 21.29	D	0
	MOTA	7675	N	ARG	320	1.860	-76.382	145.597	1.00 22.22	D	N
	MOTA	7676	CA	ARG	320	3.025	-77.044	146.163	1.00 23.46	D	С
	MOTA	7677	CB	ARG	320	3.699	-77.913	145.100	1.00 25.91	D	C
30	ATOM	7678	CG	ARG	320	4.765	-78.840	145.639	1.00 29.09	D	С
	MOTA	7679	CD	ARG	320	4.173	-79.913	146.542	1.00 32.17	D	С
	MOTA	7680	NE	ARG	320	5.219	-80.808	147.039	1.00 35.46	D	N
	ATOM	7681	CZ	ARG	320	5.452	-82.041	146.590	1.00 35.28	D	С
0.5	MOTA	7682	NH1	ARG	320	4.712	-82.566	145.619	1.00 35.19	D	N
35	ATOM	7683	NH2	ARG	320	6.439	-82.752	147.120	1.00 36.23	D	N
	MOTA	7684	С	ARG	320	4.003	-75.985	146.675	1.00 22.95	D	C
	MOTA	7685	0	ARG	320	4.571	-76.127	147.758	1.00 22.89	D	0
	MOTA	7686	N	SER	321	4.208	-74.929	145.893	1.00 22.56	D	N
40	MOTA	7687	CA	SER	321			146.302	1.00 23.16	D	С
40	MOTA	7688	СВ	SER	321			145.210	1.00 24.44	D	C
	MOTA	7689	OG	SER	321			144.004	1.00 29.71	D	0
	ATOM	7690	С	SER	321			147.578	1.00 21.76	D	•
	MOTA	7691	0	SER	321			148.477	1.00 21.35	D	0
45	ATOM	7692	N	ILE	322			147.648	1.00 20.52	D	N
45	MOTA	7693	CA	ILE	322			148.825	1.00 20.27	D	С
	MOTA	7694	CB	ILE	322			148.611	1.00 19.98	D	С
	MOTA	7695		ILE	322			7 149.941	1.00 20.29	D	C
	MOTA	7696		ILE	322			7 147.601	1.00 20.19	D	С
	ATOM	7697		ILE	322			l 147.197	1.00 21.36	D	С
50	MOTA	7698	С	ILE	322			5 150.054	1.00 19.11	D	С
	MOTA	7699		ILE	322			2 151.120	1.00 17.80	D	0
	MOTA	7700		ASN	323			1 149.888	1.00 20.09	D	N
	MOTA	7701		ASN	323			1 150.972	1.00 20.89	D	C
EF	ATOM	7702		ASN	323			7 150.449		D	С
55	MOTA	7703		ASN	323			1 151.556		D	С
	MOTA	7704		LASN	323			2 151.453		D	-
	MOTA	7705		2 ASN	323			3 152.602		D	
	MOTA	7706	С	ASN	323	4.398	3 -75.36	9 151.511	1.00 20.52	D	С

-302-

	MOTA	7707		ASN	323			152.718	1.00 18.86	D	0
	MOTA	7708		GLU	324			150.610	1.00 20.84	D	N
	MOTA	7709		GLU	324		-74.997		1.00 22.21	D	C
_	MOTA	7710		GLU	324		-75.077		1.00 23.95	D	C
5	MOTA	7711		GLU	324		-76.472		1.00 27.94	D	С
	MOTA	7712		GLU	324			148.003	1.00 31.05	D	C
	MOTA	7713	OE1		324		-75.663		1.00 33.20	D	0
	ATOM	7714		GLU	324			147.435	1.00 32.71	D	0
4.0	MOTA	7715		GLU	324			151.671	1.00 21.32	D	C
10	MOTA	7716		GLU	324			152.633	1.00 20.59	D	0
	MOTA	7717		ALA	325			151.140	1.00 20.62	D	N
	MOTA	7718		ALA	325			151.707	1.00 20.95	D	С
	MOTA	7719		ALA	325			150.853	1.00 20.62	D	C
	MOTA	7720	C	ALA	325			153.139	1.00 21.67	D	С
15	MOTA	7721	0	ALA	325			154.002	1.00 23.20	D	0
	MOTA	7722	N	TYR	326			153.396	1.00 21.72	D	N
	MOTA	7723	CA	TYR	326	4.259	-72.285	154.747	1.00 22.87	D	C
	MOTA	7724	CB	TYR	326	3.150	-73.337	154.798	1.00 21.37	D	C
	MOTA	7725	CG	TYR	326	1.745	-72.783	154.727	1.00 20.49	D	С
20	ATOM	7726	CD1	TYR	326	1.246	-71.948	155.730	1.00 19.50	D	C
	MOTA	7727	CE1	TYR	326			155.701	1.00 18.19	D	C
	MOTA	7728	CD2	TYR	326	0.889	-73.145	153.689	1.00 19.15	D	C
	MOTA	7729	CE2	TYR	326	-0.422	-72.707	153.652	1.00 17.68	D	C
	MOTA	7730	CZ	TYR	326			154.658	1.00 18.08	D	С
25	MOTA	7731	OH	TYR	326	-2.220	-71.494	154.626	1.00 16.91	D	0
	MOTA	7732	С	TYR	326	5.392	-72.697	155.688	1.00 23.78	D	C
	MOTA	7733	0	TYR	326	5.551	-72.135	156.775	1.00 22.86	D	0
	MOTA	7734	N	GLY	327	6.173	-73.687	155.263	1.00 24.36	D	N
	MOTA	7735	CA	GLY	327	7.298	-74.147	156.064	1.00 25.31	D	C
30	MOTA	7736	С	GLY	327	8.252	-73.007	156.385	1.00 26.49	D	С
	MOTA	7737	0	GLY	327	8.747	-72.901	157.504	1.00 26.84	D	0
	MOTA	7738	N	TYR	328	8.518	-72.150	155.406	1.00 27.41	D	N
	MOTA	7739	CA	TYR	328			155.623	1.00 28.77	D	C
	MOTA	7740	CB	TYR	328	9.628	-70.263	154.306	1.00 30.90	D	C
35	MOTA	7741	CG	TYR	328			154.434	1.00 33.99	D	C
	MOTA	7742	CD1		328			154.311	1.00 35.76	D	С
	MOTA	7743	CE1		328			154.423	1.00 37.49	D	C
	MOTA	7744	CD2		328			154.676	1.00 35.90	D	С
	MOTA	7745	CE2		328			154.793	1.00 36.85	D	С
40	MOTA	7746	cz	TYR	328			154.664	1.00 38.17	D	С
	MOTA	7747	OH	TYR	328			154.779	1.00 38.64	D	0
	MOTA	7748	C	TYR	328			156.652		D	
	MOTA	7749	0	TYR	328			157.585	1.00 28.57	D	0
4-	MOTA	7750	N	GLN	329			156.479	1.00 27.87	D	N
45	MOTA	7751	CA	GLN	329			157.402	1.00 27.72	D	С
	MOTA	7752	CB	GLN	329			157.005	1.00 26.32	D	C
	MOTA	7753	CG	GLN	329			155.609	1.00 24.53	D	С
	MOTA	7754	CD	GLN	329			2 155.502	1.00 24.96	D	С
	MOTA	7755		GLN	329			3 154.711	1.00 24.59	D	0
50	MOTA	7756		GLN	329			156.295	1.00 22.57	D	N
	MOTA	7757	С	GLN	329			2 158.838	1.00 28.33	D	С
	MOTA	7758	0	GLN	329			159.761	1.00 27.55	D	0
	MOTA	7759	N	ILE	330			9 159.024	1.00 29.84	D	N
	MOTA	7760	CA	ILE	330			3 160.357	1.00 31.64	D	С
55	ATOM	7761	CB	ILE	330			1 160.324	1.00 31.62	D	С
	MOTA	7762		ILE	330			L 161.668		D	С
	MOTA	7763		ILE	330			7 160.000	1.00 31.78	D	С
	MOTA	7764	CD1	. ILE	330	4.216	-74.19	5 159.714	1.00 32.07	D	С

-303-

	MOTA	7765	C	ILE	330	8.081	-71.215	161.017	1.00 33.17	D	С
	MOTA	7766	0	ILE	330	8.180	-71.044	162.233	1.00 32.52	D	0
	MOTA	7767	N	GLN	331	9.142	-71.358	160.229	1.00 34.61	D	N
_	MOTA	7768	CA	GLN	331	10.489	-71.323	160.790	1.00 36.32	D	C
5	MOTA	7769	CB	GLN	331			159.885	1.00 37.97	D	C
	ATOM	7770	CG	GLN	331	11.516	-73.581	160.175	1.00 41.59	D	C
	MOTA	7771	CD	GLN	331	11.035	-74.429	159.014	1.00 44.09	D	C
	ATOM	7772	OE1	GLN	331	11.678	-74.490	157.958	1.00 45.41	D	0
	MOTA	7773	NE2	GLN	331	9.894	-75.091	159.201	1.00 45.77	D	N
10	MOTA	7774	С	GLN	331	11.033	-69.922	161.055	1.00 36.37	D	C
	MOTA	7775	0	GLN	331	11.827	-69.732	161.973	1.00 36.85	D	0
	MOTA	7776	N	HIS	332	10.590	-68.946	160.268	1.00 36.20	D	N
	MOTA	7777	CA	HIS	332	11.060	-67.569	160.399	1.00 35.92	D	C
	MOTA	7778	CB	HIS	332	11.273	-66.977	159.006	1.00 38.26	D	C
15	MOTA	7779	CG	HIS	332	12.444	-67.562	158.281	1.00 40.86	D	C
	MOTA	7780	CD2	HIS	332	12.602	-68.754	157.656	1.00 41.83	D	C
	MOTA	7781	ND1	HIS	332	13.659	-66.916	158.186	1.00 41.67	D	N
	MOTA	7782	CE1	HIS	332	14.514	-67.684	157.535	1.00 42.92	D	C
	MOTA	7783	NE2	HIS	332	13.899	-68.806	157.202	1.00 42.63	D	N
20	MOTA	7784	С	HIS	332	10.197	-66.612	161.217	1.00 34.94	D	С
	MOTA	7785	0	HIS	332	10.631	-65.502	161.523	1.00 34.73	D	0
	MOTA	7786	N	ILE	333	8.986	-67.025	161.577	1.00 33.52	D	N
	MOTA	7787	CA	ILE	333	8.103	-66.154	162.343	1.00 31.90	D	С
	MOTA	7788	CB	ILE	333	6.845	-65.815	161.524	1.00 32.25	D	C
25	MOTA	7789	CG2	ILE	333	5.909	-64.930	162.337	1.00 31.29	D	C
	ATOM	7790	CG1	ILE	333	7.260	-65.115	160.224	1.00 31.70	D	C
	MOTA	7791	CD1	ILE	333	6.134	-64.907	159.231	1.00 31.83	D	C
	ATOM	7792	С	ILE	333	7.697	-66.776	163.670	1.00 31.12	D	C
	ATOM	7793	0	ILE	333	6.922	-67.729	163.707	1.00 30.47	D	0
30	MOTA	7794	N	GLN	334	8.230	-66.233	164.762	1.00 30.13	D	N
	MOTA	7795	CA	GLN	334	7.917	-66.747	166.092	1.00 29.64	D	С
	MOTA	7796	CB	GLN	334	8.673	-65.958	3 167.171	1.00 31.35	D	С
	MOTA	7797	CG	GLN	334	8.555	-66.553	168.571	1.00 35.01	D	C
	MOTA	7798	CD	GLN	334	9.374	-65.800	169.612	1.00 38.12	D	С
35	MOTA	7799	OE1	GLN	334	9.003	-64.707	7 170.050	1.00 39.79	D	0
	MOTA	7800	NE2	GLN	334	10.499	-66.383	170.009	1.00 40.23	D	N
	MOTA	7801	С	GLN	334	6.420	-66.670	166.366	1.00 27.88	D	C
	MOTA	7802	0	GLN	334	5.783	-65.647	7 166.115	1.00 25.92	D	0
	MOTA	7803	N	GLY	335	5.861	-67.763	3 166.871	1.00 26.57	D	N
40	ATOM	7804	CA	GLY	335	4.445	-67.785	5 167.186	1.00 25.42	D	C
	ATOM	7805	С	GLY	335	3.539	-68.439	9 166.159	1.00 23.73	D	C
	MOTA	7806	0	GLY	335	2.503	-68.97	7 166.525	1.00 22.96	D	0
	MOTA	7807	N	LEU	336			164.883	1.00 23.02	D	N
	MOTA	7808	CA	LEU	336			5 163.855	1.00 23.83	D	С
45	MOTA	7809	СВ	LEU	336	3.673	-68.812	2 162.465	1.00 24.18		С
	MOTA	7810	CG	LEU	336			9 161.718	1.00 25.08		С
	MOTA	7811		LEU	336			9 160.312	1.00 25.55		С
	MOTA	7812		LEU	336			6 161.640	1.00 23.47		
	MOTA	7813	С	LEU	336			0 164.084	1.00 24.21		_
50	ATOM	7814	0	LEU	336			8 163.814	1.00 23.84		_
	MOTA	7815	N	SER	337			1 164.578	1.00 24.29		
	ATOM	7816		SER	337			4 164.827	1.00 25.75		_
	MOTA	7817		SER	337			3 165.388	1.00 26.85		_
	MOTA	7818		SER	337	5.392		9 166.625			_
55	MOTA	7819		SER	337	2.638		6 165.786			_
	MOTA	7820		SER	337			6 165.773			_
	MOTA	7821		ALA	338			0 166.625			
	MOTA	7822	CA	ALA	338	1.138	8 -72.27	2 167.556	1.00 26.59	D	С

-304-

					220	0 000 71 000 160 410 1 00	26 05	_	^
	ATOM	7823		ALA	338		26.85 27.29	D D	C
	MOTA	7824		ALA	338				
	MOTA	7825		ALA	338		27.76	D	0
_	MOTA	7826		MET	339		27.52	D	N
5	ATOM	7827	-	MET	339		29.68	D	C
	MOTA	7828		MET	339		26.75	D	C
	MOTA	7829		MET	339		24.80	D	C
	MOTA	7830		MET	339		21.82	D	S
	MOTA	7831	CE	MET	339		22.13	D	C
10	ATOM	7832	C	MET	339		32.16	D	С
	ATOM	7833	0	MET	339	2.268 -74.263 163.271 1.00	32.08	D	0
	ATOM	7834	N	MET	340	0.204 -74.574 164.087 1.00	36.22	D	N
	MOTA	7835	CA	MET	340	0.037 -75.858 163.409 1.00	41.37	D	C
	MOTA	7836	CB	MET	340	1.340 -76.439 163.713 1.00	42.92	D	C
15	MOTA	7837	CG	MET	340	2.436 -75.849 162.858 1.00	45.73	D	C
	ATOM	7838	SD	MET	340	2.720 -76.818 161.366 1.00	51.37	D	S
	ATOM	7839	CE	MET	340		49.14	D	С
	ATOM	7840	C	MET	340		43.73	D	C
	ATOM	7841	Ö	MET	340		44.25	D	0
20	ATOM	7842	N	PRO	341		46.50	D	N
	MOTA	7843	CD	PRO	341		47.23	D	C
	MOTA	7844	CA	PRO	341		49.23	D	Č
	ATOM	7845	СВ	PRO	341		48.42	D	C
	ATOM	7846	CG	PRO	341		47.95	D	Č
25	ATOM	7847	C	PRO	341		51.91	D	Ċ
20	ATOM	7848	Ö	PRO	341		52.98	Ď	ō
	MOTA	7849	N	LEU	342		54.46	D	N
	ATOM	7850	CA	LEU	342		56.95	D	Ĉ
	ATOM	7851	CB	LEU	342		57.06	D	č
30	ATOM	7852	CG	LEU	342		57.17	D	č
00	MOTA	7853		LEU	342		57.93	D	č
	ATOM	7854		LEU	342		57.79	D	Č
	ATOM	7855	C	LEU	342		58.67	D	Č
	ATOM	7856	Ö	LEU	342		58.76	D	ŏ
35	ATOM	7857	N	LEU	343		60.38	D	N
00	ATOM	7858	CA	LEU	343		0 62.04	D	Ċ
	ATOM	7859	CB	LEU	343		0 61.76	Ď	č
	ATOM	7860	CG	LEU	343		0 61.24	D	č
	ATOM	7861		LEU	343	-0.183 -82.777 170.236 1.0		D	Č
40	ATOM	7862		LEU	343		0 61.07	D	c
40	ATOM	7863	C	LEU	343		0 63.41	D	c
	ATOM	7864		LEU	343		0 63.91	D	ŏ
		7865	-	GLN	344		0 64.75	D	N
	ATOM	7866		GLN	344		0 66.45	D	C
45	ATOM				344		0 66.30	D	č
40	ATOM	7867		GLN	344		0 65.84	D	C
	ATOM	7868		GLN	344		0 65.57	D	c
	ATOM	7869		GLN			0 65.72	D	Ö
	MOTA	7870			344		0 65.11	D	N
50	ATOM	7871			344		0 67.47	D	
50	ATOM	7872		GLN	344		0 67.50	D	C
	ATOM	7873		GLN	344		0 68.16	D	0
	ATOM	7874		GLU	345				N
	MOTA	7875		GLU	345		0 69.15	D	C
	MOTA	7876		GLU	345		0 69.28	D	С
55	MOTA	7877		GLU	345		0 69.98		C
	MOTA	7878		GLU	345		0 70.48		
	MOTA	7879		l GLU	345		0 70.72		-
	MOTA	7880) OE	2 GLU	345	4.944 -77.996 162.651 1.0	0 70.76	D	0

-305-

	ATOM	7881	С	GLU	345			161.585	1.00 69.56	D	С
	ATOM	7882	0	GLU	345			160.466	1.00 69.53	D	0
	MOTA	7883	N	ILE	346			162.505	1.00 69.54	D	N
_	MOTA	7884	CA	ILE	346	0.306	-83.292	162.333	1.00 70.13	D	C
5	MOTA	7885	CB	ILE	346	0.604	-84.111	161.035	1.00 69.60	D	C
	ATOM	7886	CG2	ILE	346	1.800	-85.036	161.268	1.00 69.36	D	C
	MOTA	7887	CG1	ILE	346	-0.642	-84.897	160.590	1.00 68.80	D	C
	MOTA	7888	CD1	ILE	346	-0.930	-86.167	161.379	1.00 67.66	D	C
	MOTA	7889	С	ILE	346	0.462	-84.208	163.552	1.00 70.49	Ð	С
10	MOTA	7890	0	ILE	346	1.504	-84.095	164.233	1.00 71.08	D	0
	MOTA	7891	OXT	ILE	346	-0.443	-85.029	163.815	1.00 71.20	D	0
	TER	7892		ILE	346					D	
	MOTA	7893	0	HOH	100	1.194-	100.903	157.437	1.00 32.35	S	0
	MOTA	7894	0	HOH	101	5.789-	101.495	107.858	1.00 41.67	S	0
15	MOTA	7895	0	HOH	102	-3.286-	100.790	155.260	1.00 35.57	S	0
	MOTA	7896	0	нон	103	-8.930-	101.202	133.287	1.00 48.12	S	0
	MOTA	7897	0	HOH	105	9.943-	103.811	110.611	1.00 44.28	S	0
	MOTA	7898	0	HOH	109	7.852	-54.504	152.498	1.00 13.54	S	0
	MOTA	7899	0	HOH	110	1.851	-59.616	158.936	1.00 15.42	S	0
20	MOTA	7900	0	нон	111	4.061	-55.748	105.937	1.00 14.89	S	0
	MOTA	7901	0	нон	112	-3.981	-55.392	158.482	1.00 12.72	S	0
	ATOM	7902	0	нон	113	-8.499	-61.621	167.958	1.00 13.73	S	0
	MOTA	7903	0	нон	114	-12.236	-61.051	158.803	1.00 15.08	S	0
	MOTA	7904	0	нон	115	-0.076	-79.912	152.707	1.00 21.70	s	0
25	MOTA	7905	0	HOH	116	-18.234	-71.054	169.058	1.00 16.92	S	0
	ATOM	7906	0	HOH	117	8.261	-61.905	96.377	1.00 18.79	S	0
	MOTA	7907	0	HOH	118	-9.485	-73.341	172.175	1.00 20.25	S	0
	ATOM	7908	0	нон	119	-12.684	-59.785	167.173	1.00 18.75	S	0
	ATOM	7909	0	нон	120	-21.219	-81.799	152.446	1.00 17.61	S	0
30	MOTA	7910	0	нон	121	-10.313	-78.143	167.136	1.00 17.35	S	0
	ATOM	7911	0	HOH	122			171.689	1.00 20.99	S	0
	MOTA	7912	0	нон	123	-7.757	-54.292	111.662	1.00 17.89	S	0
	MOTA	7913	0	нон	124	-16.140	-46.485	114.634	1.00 19.91	S	0
	MOTA	7914	0	нон	125	5.487	-53.523	168.579	1.00 16.20	S	0
35	MOTA	7915	0	HOH	126	12.646	-74.069	123.673	1.00 19.14	S	0
	MOTA	7916	0	HOH	127	14.789	-87.134	104.722	1.00 18.59	S	0
	ATOM	7917	0	HOH	128	-1.875	-59.315	105.692	1.00 19.91	S	0
	ATOM	7918	0	HOH	129	-11.949	-41.023	122.709	1.00 19.77	S	0
	ATOM	7919	0	HOH	130	-9.684	-54.904	96.052	1.00 20.41	S	0
40	ATOM	7920	0	нон	131	-9.323	-60.374	151.871	1.00 19.86	S	0
	ATOM	7921	0	нон	132	-11.101	-60.624	169.075	1.00 18.09	S	0
	ATOM	7922	0	HOH	133	-16.739	-45.232	95.584	1.00 22.60	s	0
	ATOM	7923	0	нон	134	18.286	-72.825	104.279	1.00 20.39	S	0
	MOTA	7924	0	HOH	135	-4.303	-46.906	5 168.333	1.00 22.87	S	0
45	MOTA	7925	0	HOH	137	-10.988	-71.168	3 169.786	1.00 25.18	S	0
	MOTA	7926	0	нон	. 138	-9.260	-59.172	2 170.779	1.00 18.48	S	0
	MOTA	7927	0	нон	139	17.621	-68.755	5 116.205	1.00 18.82	S	0
	ATOM	7928	0	нон	140	-1.448	-79.558	3 111.697	1.00 22.23	S	0
	ATOM	7929	0	нон	141	-18.854	-71.09	7 159.796	1.00 19.71	S	0
50	MOTA	7930	0	нон	142	-5.714	-58.929	9 112.169	1.00 20.72	S	0
	ATOM	7931	0	нон	143		-46.85		1.00 25.75	S	0
	ATOM	7932		нон	144			8 156.566	1.00 21.61	S	0
	ATOM	7933		нон	145			2 163.145	1.00 18.35	S	0
	ATOM	7934		нон	146			3 140.426	1.00 21.72	s	ō
55	ATOM	7935		нон	147			3 141.695	1.00 18.66	s	
_	ATOM	7936		нон	148			B 103.032	1.00 16.53	s	
	ATOM	7937		нон	149			4 117.113	1.00 23.48	s	
	ATOM	7938		нон	150			5 161.564		S	
			-				_				

-306-

	ATOM	7939	0	нон	151		-53.158		1.00 17.95		0
	MOTA	7940	0	нон	152		-59.391		1.00 19.34		0
	MOTA	7941	0	нон	153		-55.938		1.00 19.01		0
_	MOTA	7942	0	нон	154		-61.052		1.00 19.61	S	0
5	MOTA	7943	0	HOH	155		-61.077		1.00 18.36	S	0
	MOTA	7944	0	нон	156			112.685	1.00 20.71	S	0
	MOTA	7945	0	нон	157			152.635	1.00 21.17	S	0
	MOTA	7946	0	HOH	158	-12.998			1.00 22.19	S	0
40	MOTA	7947	0	НОН	159	-10.033			1.00 26.61	S	0
10	MOTA	7948	0	нон	160	-14.613			1.00 21.46	S	0
	MOTA	7949	0	HOH	161		-59.730	96.207	1.00 22.15	S	0
	MOTA	7950	0	нон	162			119.289	1.00 25.62	S	0
	MOTA	7951	0	нон	163			155.101	1.00 24.72	S	0
45	MOTA	7952	0	HOH	164			149.752	1.00 24.52	S	0
15	MOTA	7953	0	HOH	165			132.956	1.00 26.75	S	0
	MOTA	7954	0	HOH	166		-73.450	91.962	1.00 24.27	S	0
	MOTA	7955	0	HOH	167		-61.210	92.554	1.00 19.81	S	0
	MOTA	7956	0	нон	168			163.877	1.00 22.12	S	0
	MOTA	7957	0	нон	169		-55.410		1.00 22.34	S	0
20	MOTA	7958	0	HOH	170			136.548	1.00 25.65	S	0
	MOTA	7959	0	HOH	171			151.754	1.00 21.47	S	0
	MOTA	7960	0	HOH	172			109.182	1.00 20.87	S	0
	MOTA	7961	0	HOH	173			109.157	1.00 22.25	S	0
05	MOTA	7962	0	нон	174			154.270	1.00 32.11	S	0
25	MOTA	7963	0	нон	175			160.770	1.00 22.21	S	0
	MOTA	7964	0	HOH	176		-68.265		1.00 22.03	S	0
	MOTA	7965	0	нон	177			134.429	1.00 33.35	S	0
	MOTA	7966	0	нон	178			109.544	1.00 26.39	S	0
20	MOTA	7967	0	НОН	179			136.264	1.00 25.98	S	0
30	MOTA	7968	0	нон	180		-55.715		1.00 21.71	S	0
	MOTA	7969	0	нон	181			170.157	1.00 21.79	S	0
	MOTA	7970	0	НОН	182			149.857	1.00 29.11	S	0
	MOTA	7971	0	НОН	183			127.493	1.00 22.42	S	0
25	ATOM	7972	0	НОН	184			111.356	1.00 24.87	S	0
35	ATOM	7973	0	НОН	185			100.449	1.00 23.13	S	0
	ATOM	7974	0	НОН	186			158.577	1.00 22.53	S	0
	ATOM	7975	0	нон	187			106.554	1.00 23.92	S	0
	MOTA	7976	0	нон	188			171.929	1.00 27.84	s	0
40	ATOM	7977	0	НОН	189			149.767	1.00 22.64	S	0
40	ATOM	7978	0	НОН	190			156.796	1.00 24.25	S	0
	ATOM	7979	0	нон	191			168.198	1.00 26.75	S	0
	ATOM	7980	0	нон	192			114.378		S	
	ATOM	7981	0	НОН	193			168.792	1.00 27.62	S	0
45	ATOM	7982	0	НОН	194			100.278	1.00 23.15	S	0
40	MOTA	7983	0	НОН	195			170.758 101.942	1.00 21.29	S	0
	ATOM	7984	0	НОН	196				1.00 26.44	s s	0
	ATOM	7985	0	НОН	197		-62.102	3 122.107	1.00 23.98		0
	ATOM	7986	0	HOH	198 199			170.098	1.00 26.12	s s	0
50	MOTA	7987	0	НОН	200				1.00 28.03 1.00 28.11	S	0
30	MOTA	7988		HOH	201		-47.303	3 95.880 7 102.862	1.00 28.11	S	0
	MOTA	7989		HOH							0
	ATOM	7990		нон	202		-58.973		1.00 25.62	S	0
	MOTA	7991	0	HOH	203			2 164.661	1.00 25.82 1.00 24.54	s s	0
55	ATOM	7992		HOH	204			144.845		S	0
JJ	ATOM	7993		HOH	205			7 147.929 3 94.498		S	0
	MOTA	7994		HOH	207		-53.97;			S	0
	MOTA	7995		HOH	208			9 169.964		S	0
	MOTA	7996	0	нон	209	2.796	-33.26	7 111.786	1.00 27.64	۵	0

-307-

	MOTA	7997	0	нон	210		-78.801		1.00 24.54		0
	MOTA	7998	0	HOH		-18.964	-44.018	109.109	1.00 21.20		0
	MOTA	7999	0	HOH	212	-17.685	-		1.00 27.48		0
_	MOTA	8000	0	нон	213		-89.525		1.00 28.97		0
5	MOTA	8001	0	HOH	214		-58.041		1.00 34.69		0
	MOTA	8002	0	HOH		-15.068			1.00 27.99	S	0
	MOTA	8003	0	нон	216	-18.184			1.00 20.26	S	0
	MOTA	8004	0	HOH	217	-5.170	-78.598	128.888	1.00 25.97	S	0
	ATOM	8005	0	HOH	218	8.686	-78.683	97.186	1.00 27.25	S	0
10	MOTA	8006	0	HOH	219	7.141	-79.540	135.217	1.00 21.04	S	0
	MOTA	8007	0	HOH	220		-46.341		1.00 21.84	S	0
	MOTA	8008	0	HOH	221		-13.878		1.00 29.72	S	0
	MOTA	8009	0	HOH	222	9.453	-32.021	164.111	1.00 23.90	S	0
	MOTA	8010	0	HOH	223		-18.447		1.00 21.15	S	0
15	MOTA	8011	0	HOH	224		-76.779		1.00 23.30	S	0
	MOTA	8012	0	HOH	225	-10.762	-67.817	169.854	1.00 25.60	S	0
	MOTA	8013	0	HOH	226	-8.111	-57.123	110.725	1.00 25.49	S	0
	ATOM	8014	0	HOH	227			169.157	1.00 27.54	S	0
	MOTA	8015	0	нон	228	-14.901	-61.518	170.186	1.00 26.01	S	0
20	ATOM	8016	0	нон	229	-12.533	-51.396	163.830	1.00 24.68	S	0
	ATOM	8017	0	нон	230	-7.243	-33.221	149.831	1.00 27.89	S	0
	MOTA	8018	0	нон	231	9.051	-59.422	93.575	1.00 25.99	S	0
	MOTA	8019	Ō	нон	232	-1.525	-42.199	127.967	1.00 28.31	S	0
	ATOM	8020	0	нон	233	-6.126	-55.469	92.922	1.00 24.15	S	0
25	ATOM	8021	0	нон	234	10.308	-22.755	159.042	1.00 24.72	S	0
	ATOM	8022	Ō	нон	235	-11.576	-58.094	151.433	1.00 35.81	S	0
	ATOM	8023	0	нон	236	-10.101	-53.349	104.435	1.00 29.28	S	0
	ATOM	8024	0	нон	237	12.619	-60.351	97.081	1.00 22.39	S	0
	ATOM	8025	O	нон	238	15.329	-43.209	142.529	1.00 25.98	s	0
30	ATOM	8026	0	нон	239	1.005	-54.014	92.643	1.00 28.69	S	0
	ATOM	8027	Ō	нон	240	14.968	-36.448	134.614	1.00 27.47	S	0
	ATOM	8028	0	нон	241	7.889	-69.278	128.039	1.00 25.45	S	0
	ATOM	8029	0	нон	242	1.344	-56.173	94.149	1.00 25.84	S	0
	ATOM	8030	0	нон	243	-13.791	-43.127	93.512	1.00 31.21	S	0
35	ATOM	8031	0	нон	244	11.904	-53.435	171.337	1.00 24.49	S	0
	MOTA	8032	0	нон	245	6.729	-70.309	164.313	1.00 26.33	S	0
	ATOM	8033	0	HOH	246	11.002	-83.852	100.804	1.00 35.04	S	0
	ATOM	8034	0	HOH	247	15.286	-72.468	123.050	1.00 27.65	S	0
	MOTA	8035	0	HOH	248	-0.135	-80.031	144.939	1.00 33.14	S	0
40	ATOM	8036	0	HOH	249	-12.834	-28.015	103.311	1.00 25.83	S	0
	ATOM	8037	0	HOH	250			149.641	1.00 32.57	S	0
	MOTA	8038	0	HOH	251			3 153.382	1.00 27.18	S	0
	MOTA	8039		HOH	252			149.250		S	0
	MOTA	8040	0	HOH	253			2 114.494			0
45	ATOM	8041	. 0	HOH	254		-63.45				0
	MOTA	8042		нон	255			3 155.492			0
	MOTA	8043	0	HOH	256			5 109.375			0
	MOTA	8044	0	HOH	257			4 153.151			0
	ATOM	8045	0	HOH	258			9 143.846			0
50	ATOM	8046	0	HOH	259			9 149.403			
	ATOM	8047		нон	260			3 161.866			
	ATOM	8048		нон	261			8 154.705			
	MOTA	8049	0	нон	263			2 156.022			
	MOTA	8050		нон	264			4 145.484			
55	ATOM	8051		нон	265			4 138.485			
	ATOM	8052		нон	266		3 -76.73				
	ATOM	8053		нон	267	7.57	3 -60.15	9 114.770	1.00 31.64		_
	ATOM	8054			268	14.54	4 -43.49	6 170.824	1.00 25.33	S	0

-308-

	MOTA	8055	0	НОН	269	-10.804	-71.018	173.076	1.00 32.63	S	0
	MOTA	8056	0	НОН	270		-62.924	146.402	1.00 29.18	S	0
	MOTA	8057	0	HOH	271	5.357	-53.638	90.691	1.00 31.79	S	0
_	MOTA	8058	0	HOH	272		-86.281		1.00 31.53	S	0
5	MOTA	8059	0	HOH	273		-19.105		1.00 29.74	S	0
	MOTA	8060	0	нон	274	-20.468	-80.759		1.00 33.49	S	0
	MOTA	8061	0	HOH	275			157.623	1.00 30.30	S	0
	MOTA	8062	0	HOH	276	15.625	-37.089	150.881	1.00 35.21	S	0
	MOTA	8063	0	HOH	277		-61.189		1.00 33.96	S	0
10	MOTA	8064	0	HOH	278		-34.573		1.00 33.68	S	0
	MOTA	8065	0	HOH	279		-47.618		1.00 28.74	S	0
	MOTA	8066	0	HOH	280		-91.753		1.00 27.73	S	0
	MOTA	8067	0	HOH	281		-44.170		1.00 31.74	S	0
	MOTA	8068	0	HOH	282		-48.188		1.00 31.25	S	0
15	MOTA	8069	0	HOH	283		-87.258		1.00 29.49	S	0
	MOTA	8070	0	HOH	284	-7.873	-59.325	161.206	1.00 27.49	S	0
	MOTA	8071	0	HOH	285	10.850	-61.174	95.346	1.00 25.49	S	0
	MOTA	8072	0	НОН	286	-9.010	-43.808	146.840	1.00 28.55	S	0
	MOTA	8073	0	нон	287		-57.925		1.00 30.97	S	0
20	MOTA	8074	0	HOH	288			107.050	1.00 31.85	S	0
	MOTA	8075	0	HOH	289			169.467	1.00 31.60	S	0
	MOTA	8076	0	HOH	290	-14.833	-96.003	155.699	1.00 35.00	S	0
	MOTA	8077	0	HOH	291			152.640	1.00 28.95	S	0
	MOTA	8078	0	HOH	292	3.887	-59.382	160.774	1.00 34.06	S	0
25	MOTA	8079	0	HOH	293	-17.158	-41.652	112.721	1.00 25.07	S	0
	MOTA	8080	0	HOH	294			160.924	1.00 37.13	S	0
	MOTA	8081	0	HOH	295			171.437	1.00 31.26	S	0
	MOTA	8082	0	HOH	296	-8.483	-70.123	175.216	1.00 31.58	S	0
~~	MOTA	8083	0	нон	297			168.111	1.00 25.65	S	0
30	MOTA	8084	0	HOH	298	1.280	-57.553	99.814	1.00 35.96	S	0
	MOTA	8085	0	HOH	299			169.041	1.00 27.46	S	0
	MOTA	8086	0	НОН	300			112.954	1.00 31.18	S	0
	ATOM	8087	0	HOH	301		-50.185		1.00 35.30	S	0
05	ATOM	8088	0	HOH	302			170.669	1.00 28.28	S	0
35	MOTA	8089	0	нон	303			127.917	1.00 33.15	S	0
	MOTA	8090	0	нон	304			112.124	1.00 35.97	S	0
	MOTA	8091	0	НОН	305			170.536	1.00 26.99	S	0
	MOTA	8092	0	нон	306		-27.751		1.00 29.26	S	0
40	ATOM	8093	0	HOH	307		-71.189		1.00 41.52	S	0
40	MOTA	8094	0	НОН	308	-2.498		102.659	1.00 41.26	S	0
	ATOM	8095	0	НОН	309			136.885	1.00 30.49	S	0
	MOTA	8096	0	НОН	310				1.00 34.52		0
	MOTA	8097	0	HOH	311			166.802	1.00 25.52	S	0
A E	ATOM	8098	0	НОН	312			123.176	1.00 29.99	S	0
45	MOTA	8099	0	НОН	313			169.043	1.00 27.78	S	0
	ATOM	8100	0	НОН	314			118.169	1.00 39.70	S	0
	ATOM	8101	0	НОН	315			177.428	1.00 40.70	S	0
	ATOM	8102	0	НОН	316			153.276	1.00 26.59	S	0
50	ATOM	8103	0	нон	317			151.565	1.00 30.90	S	0
30	ATOM	8104	0	нон	318			109.924	1.00 35.70	S	0
	ATOM	8105	0	HOH	319			167.637	1.00 27.84	S	0
	ATOM	8106	0	HOH	320			141.033	1.00 34.15	S	0
	MOTA	8107	0	HOH	321			129.073	1.00 35.91	S	0
55	MOTA	8108	0	HOH	323			108.859	1.00 40.25	S	0
J J	ATOM	8109	0	HOH	324			153.806	1.00 29.58	S	0
	MOTA	8110	0	HOH	325			148.698	1.00 38.84	S	0
	MOTA	8111	0	HOH	326			151.149	1.00 33.24	S	0
	MOTA	8112	0	нон	327	13.382	-37.762	154.701	1.00 36.77	S	0

-309-

	MOTA	8113	0	нон	328	-4.082	-52.659	145.859	1.00 35.37	S	0
	MOTA	8114	0	HOH	329	-12.214	-97.380	152.729	1.00 40.91	S	0
	MOTA	8115	0	HOH	330	21.253	-78.801	100.196	1.00 41.54	S	0
	MOTA	8116	0	HOH	331	20.349	-66.162	108.672	1.00 39.01	S	0
5	MOTA	8117	0	HOH	332	14.913	-47.738	137.531	1.00 41.04	S	0
	ATOM	8118	0	нон	333	4.138	-44.506	175.935	1.00 34.58	S	0
	MOTA	8119	0	HOH	334	-23.111	-25.163	112.021	1.00 44.12	S	0
	MOTA	8120	0	нон	335	14.393	-21.278	151.249	1.00 38.52	S	0
	MOTA	8121	0	нон	336	-7.214	-56.582	102.979	1.00 30.20	S	0
10	MOTA	8122	0	нон	337	-10.229		99.872	1.00 30.38	S	0
	MOTA	8123	0	нон	338	19.511	-44.397	155.298	1.00 29.41	S	0
	ATOM	8124	0	нон	339		-74.211	95.233	1.00 32.45	S	0
	ATOM	8125	0	нон	340	-3.916	-30.077	164.362	1.00 31.78	S	0
	ATOM	8126	O	НОН	341			105.562	1.00 28.04	S	0
15	ATOM	8127	Ō	нон	343			109.753	1.00 42.19	s	Ō
	ATOM	8128	ō	нон	344			170.396	1.00 27.91	s	ō
	MOTA	8129	ŏ	нон	345			160.678	1.00 43.95	s	ŏ
	ATOM	8130	Ö	нон	346			117.144	1.00 35.29	s	ŏ
	ATOM	8131	ŏ	нон	347			116.848	1.00 34.25	Š	ō
20	MOTA	8132	Ö	нон	348			113.302	1.00 34.77	s	ŏ
	ATOM	8133	ŏ	нон	349			145.069	1.00 31.88	S	ŏ
	ATOM	8134	ŏ	нон	350			168.903	1.00 37.36	S	ŏ
	ATOM	8135	ŏ	нон	351			153.017	1.00 37.50	S	ŏ
	ATOM	8136	ŏ	нон	352			156.021	1.00 32.52	S	Ö
25	ATOM	8137	ŏ	нон	353			145.123	1.00 26.19	S	o
20	ATOM	8138	ŏ	нон	354			166.993	1.00 20.19	S	Ö
	ATOM	8139	ŏ	нон	355			153.100	1.00 42.33	S	o
	MOTA	8140	ŏ	нон	356			173.508	1.00 30.00	S	o
	MOTA	8141	Ö	нон	358			128.237	1.00 47.01	S	0
30	ATOM	8142	ŏ	нон	359			156.601	1.00 31.19	S	o
30	ATOM	8143	0	нон	360			100.980	1.00 27.83	S	0
	ATOM	8144	0	нон	361		-36.663		1.00 27.83	S	
			0		362			149.391			0
	MOTA MOTA	8145		HOH					1.00 39.87	S	0
35		8146	0	нон	363 364			164.566	1.00 29.90	S	0
33	MOTA	8147	0	нон				135.114	1.00 32.66	S	0
	ATOM	8148	0	нон	365			157.785	1.00 32.62	S	0
	ATOM	8149	0	нон	366			109.527	1.00 39.14	S	0
	ATOM	8150	0	нон	367			159.935	1.00 30.91	S	0
40	ATOM	8151	0	нон	369			103.921	1.00 33.02	S	0
40	ATOM	8152	0	нон	370			128.744	1.00 35.96	S	0
	ATOM	8153	0	нон	371			122.607	1.00 39.74	S	0
	MOTA	8154	0	НОН	372			170.898	1.00 33.17		0
	ATOM	8155	0	НОН	373			157.889	1.00 47.16	S	0
A.E.	MOTA	8156	0	НОН	374			173.306	1.00 31.81	S	0
45	ATOM	8157	0	НОН	375			156.839	1.00 43.43	S	0
	MOTA	8158	0	НОН	376			147.266	1.00 33.03	S	0
	MOTA	8159	0	нон	377			152.019	1.00 31.07	S	0
	MOTA	8160	0	HOH	378			134.105	1.00 37.41	S	0
50	MOTA	8161	0	нон	379			157.807	1.00 44.33	S	0
50	MOTA	8162	0	нон	380			3 127.555	1.00 35.49	S	0
	MOTA	8163	0	нон	381			3 173.073	1.00 35.86	S	0
	MOTA	8164	0	нон	383			3 108.536	1.00 37.37	S	0
	MOTA	8165	0	нон	385			1 129.029	1.00 41.45	S	0
	MOTA	8166	0	HOH	386			1 105.307	1.00 44.00	s	0
55	MOTA	8167	0	HOH	387			5 164.207	1.00 37.54	S	0
	MOTA	8168	0	HOH	388			0 130.123	1.00 34.65	S	0
	MOTA	8169	0	HOH	389			5 114.570		S	0
	MOTA	8170	0	HOH	390	-2.415	-72.57	6 135.885	1.00 30.52	S	0

-310-

	ATOM	8171	0	нон	391	-8.453	-70.094	98.112	1.00 40.15	S	0
	ATOM	8172	0	HOH	392	-4.178	-80.568	127.822	1.00 31.47	S	0
	ATOM	8173	0	HOH	393	-17.842	-63.215	143.635	1.00 39.38	S	0
_	MOTA	8174	0	HOH	394	-19.264	-81.648	157.206	1.00 32.27	S	0
5	MOTA	8175	0	HOH	396	-20.956			1.00 33.04	S	0
	ATOM	8176	0	HOH	397	1.082	-45.036	161.177	1.00 36.77	S	0
	MOTA	8177	0	HOH	399	-16.486	-93.083	157.191	1.00 38.04	S	0
	MOTA	8178	0	нон	400	18.520	-69.299	94.579	1.00 38.46	S	0
	ATOM	8179	0	НОН	401	-14.376	-47.406	162.731	1.00 43.61	S	0
10	MOTA	8180	0	HOH	402	-15.725	-46.681	93.561	1.00 36.70	S	0
	MOTA	8181	0	HOH	403	15.449	-93.447	107.056	1.00 42.96	S	0
	ATOM	8182	0	нон	404	17.756	-34.951	160.597	1.00 38.74	S	0
	ATOM	8183	0	HOH	405	-11.516	-52.980	92.984	1.00 31.69	S	0
	MOTA	8184	0	нон	406	2.904	-99.028	157.874	1.00 35.56	S	0
15	MOTA	8185	0	нон	407	3.990	-47.232	174.280	1.00 54.42	S	0
	MOTA	8186	0	нон	408	5.363	-82.052	150.581	1.00 39.03	S	0
	MOTA	8187	0	HOH	409	-13.329	-21.194	112.697	1.00 38.48	S	0
	MOTA	8188	0	HOH	410	-20.132	-46.572	109.024	1.00 42.34	S	0
	ATOM	8189	0	нон	411	-20.146	-71.594	142.398	1.00 48.84	S	0
20	ATOM	8190	0	HOH	413	7.810	-96.588	117.307	1.00 48.54	S	0
	MOTA	8191	0	нон	414	-15.707	-39.444	112.856	1.00 30.16	S	0
	ATOM	8192	0	нон	415	-7.705	-43.981	141.677	1.00 42.54	S	0
	MOTA	8193	0	нон	416	-11.327	-80.716	166.581	1.00 29.92	S	0
	MOTA	8194	0	нон	417	14.765	-15.174	132.791	1.00 46.34	S	0
25	MOTA	8195	0	нон	418	12.180	-35.626	148.220	1.00 43.95	S	0
	ATOM	8196	0	нон	419	-0.687	-69.344	171.152	1.00 37.41	S	0
	ATOM	8197	0	нон	420	-11.442	-58.044	158.798	1.00 36.92	S	0
	MOTA	8198	0	нон	421	12.102	-62.691	93.583	1.00 34.13	S	0
	MOTA	8199	0	нон	422		-38.085		1.00 52.29	S	0
30	ATOM	8200	O	нон	423	12.749	-96.511	113.885	1.00 39.83	S	0
	ATOM	8201	0	нон	424	2.752	-31.848	124.578	1.00 44.26	S	0
	MOTA	8202	0	нон	425			112.133	1.00 44.28	S	0
	ATOM	8203	0	нон	427	-10.440	-68.616	172.311	1.00 32.78	S	0
	ATOM	8204	0	нон	428	-6.952	-47.164	90.926	1.00 36.61	S	0
35	ATOM	8205	0	нон	429	-5.052	-57.339	148.491	1.00 39.32	S	0
	ATOM	8206	0	HOH	431	-1.897	-61.286	90.062	1.00 52.91	S	0
	ATOM	8207	0	нон	432	17.295	-72.124	95.247	1.00 51.20	S	0
	MOTA	8208	0	нон	433	-8.442	-44.268	167.166	1.00 38.87	S	0
	MOTA	8209	0	нон	434	17.130	-51.752	145.075	1.00 37.31	S	0
40	MOTA	8210	0	нон	435	-11.934	-41.853	89.278	1.00 35.15	S	0
	MOTA	8211	0	HOH	436	-20.655	-79.110	158.422	1.00 38.37	S	0
	ATOM	8212	0	HOH	437	-17.692	-58.619	152.324	1.00 39.50	S	0
	ATOM	8213	0	нон	438	-13.228	-92.072	160.458	1.00 42.10	S	0
	ATOM	8214		HOH	439	4.172	-12.941	153.839	1.00 33.74	S	0
45	ATOM	8215		нон	440	-10.145	-87.720	162.303	1.00 38.35	S	0
	ATOM	8216		HOH	442	-10.931	-61.150	93.207	1.00 45.01	S	0
	ATOM	8217		нон	443	-1.358	-40.495	93.770	1.00 37.78	S	0
	ATOM	8218		нон	446	-6.450	-68.499	9 173.937	1.00 37.62	S	0
	MOTA	8219		нон	448	24.212	-70.50	5 107.734	1.00 48.81	S	0
50	MOTA	8220		нон	449	-6.596	-43.86	93.009	1.00 32.44	S	0
	ATOM	8221		нон	450			3 142.094		S	0
	MOTA	8222		НОН	452			8 155.435		S	0
	ATOM	8223		нон	453			7 111.600		S	0
	ATOM	8224		нон	454			2 142.327		S	0
55	ATOM	8225		нон	455			7 174.211		s	
-	ATOM	8226		нон	456			9 117.025		S	
	ATOM	8227		нон	458			5 151.820		S	
	ATOM	8228			459			7 143.893		S	

-311-

	MOTA	8229	0	НОН	461	-12.126 -			1.00 53.95	S	0
	MOTA	8230	0	НОН	462		-12.385		1.00 34.36	S	0
	MOTA	8231	0	HOH	463		-61.641		1.00 42.87	S	0
_	MOTA	8232	0	нон	464		-88.839		1.00 51.28	S	0
5	MOTA	8233	0	нон	465		-57.821		1.00 39.77	S	0
	MOTA	8234	0	HOH	466		-70.873		1.00 43.43	S	0
	MOTA	8235	0	нон	467		-61.794	90.011	1.00 43.72	S	0
	MOTA	8236	0	нон	468		-18.321		1.00 44.03	S	0
	MOTA	8237	0	нон	469		-34.938		1.00 37.93	S	0
10	MOTA	8238	0	HOH	470		-	108.828	1.00 47.92	S	0
	MOTA	8239	0	HOH	472	-4.726	-64.694	95.196	1.00 35.25	S	0
	ATOM	8240	0	HOH	473	-22.754			1.00 34.93	S	0
	ATOM	8241	0	HOH	474			120.698	1.00 34.05	S	0
	MOTA	8242	0	HOH	475	-10.065			1.00 42.11	S	0
15	MOTA	8243	0	HOH	476			110.275	1.00 38.54	S	0
	MOTA	8244	0	HOH	477	16.699	-92.866	125.208	1.00 39.15	S	0
	ATOM	8245	0	HOH	478	-8.371	-55.088	161.316	1.00 43.44	S	0
	MOTA	8246	0	HOH	479	-10.360	-72.131	177.271	1.00 57.30	S	0
	MOTA	8247	0	HOH	481	-10.827	-16.909	116.124	1.00 45.61	S	0
20	MOTA	8248	0	HOH	483	3.497	-28.876	114.517	1.00 38.30	S	0
	MOTA	8249	0	HOH	485	16.708	-79.915	98.646	1.00 36.18	S	0
	MOTA	8250	0	HOH	486	5.685	-70.865	142.719	1.00 39.47	S	0
	MOTA	8251	0	HOH	487			115.024	1.00 44.49	S	0
	MOTA	8252	0	HOH	489	8.085	-58.272	171.632	1.00 41.31	S	0
25	MOTA	8253	0	HOH	490	-23.161			1.00 53.30	S	0
	MOTA	8254	0	HOH	491	5.795	-69.729	129.532	1.00 41.18	S	0
	MOTA	8255	0	HOH	492			154.533	1.00 36.96	S	0
	ATOM	8256	0	HOH	493	9.143	-81.316	97.155	1.00 35.88	S	0
	MOTA	8257	0	HOH	494			121.694	1.00 33.42	S	0
30	MOTA	8258	0	HOH	495	9.282	-47.550	112.568	1.00 35.91	S	0
	MOTA	8259	0	HOH	496	13.335	-57.030	154.593	1.00 47.05	S	0
	MOTA	8260	0	HOH	497			148.612	1.00 39.22	S	0
	MOTA	8261	0	HOH	498	-10.245	-19.394	103.261	1.00 39.63	S	0
	MOTA	8262	0	HOH	499	-14.636	-36.366	113.518	1.00 34.44	S	0
35	MOTA	8263	0	HOH	500	-11.669	-46.517	135.894	1.00 47.58	S	0
	MOTA	8264	0	HOH	501	11.046	-44.408	115.223	1.00 39.61	S	0
	ATOM	8265	0	HOH	502			124.095	1.00 51.93	S	0
	MOTA	8266	0	HOH	503			140.453	1.00 46.40	S	0
	ATOM	8267	0	HOH	504			134.440	1.00 46.55	S	0
40	MOTA	8268	0	HOH	505		-68.377		1.00 46.90	S	0
	ATOM	8269	0	HOH	506			108.740	1.00 42.45	S	0
	MOTA	8270		HOH	508			153.730		S	_
	ATOM	8271	0	HOH	509			107.564	1.00 43.38	S	0
45	MOTA	8272	0	нон	510			155.934	1.00 48.47	S	0
45	MOTA	8273	0	HOH	511			135.988	1.00 43.55	S	0
	MOTA	8274	0	нон	512			114.704	1.00 39.28	S	0
	MOTA	8275	0	нон	513			157.603	1.00 42.13	S	0
	MOTA	8276	0	нон	514			143.859	1.00 48.19	S	0
	MOTA	8277	0	HOH	515			113.699	1.00 41.10	S	0
50	MOTA	8278		нон	516			162.242	1.00 53.03	S	0
	ATOM	8279		HOH	517			120.083	1.00 50.51	S	0
	ATOM	8280		нон	518			158.553	1.00 34.18	S	
	MOTA	8281		нон	519		-65.958		1.00 37.35	S	
	MOTA	8282		нон	520			158.067	1.00 40.43	S	
55	MOTA	8283		HOH	521			107.777	1.00 34.60	S	
	MOTA	8284		нон	523		-57.467		1.00 44.57	S	
	MOTA	8285			524			104.702	1.00 49.92	S	
	MOTA	8286	0	HOH	525	23.766	-78.865	111.717	1.00 49.25	S	0

-312-

	ATOM	8287	0	нон	526	12.535	-38.204	148.153	1.00 53.45	Ş	0
	MOTA	8288	0	нон	527	-6.678	-65.953	114.241	1.00 45.88		0
	MOTA	8289	0	HOH	529	-21.878	-58.439	164.200	1.00 48.19	S	0
_	MOTA	8290	0	HOH	530	-11.825	-37.756	116.383	1.00 45.97	S	0
5	MOTA	8291	0	HOH	532	-11.859	-61.199	109.587	1.00 49.73		0
	MOTA	8292	0	HOH	533		-38.372		1.00 43.27		0
	MOTA	8293	0	HOH	535	-9.521	-45.912	129.467	1.00 40.80		0
	MOTA	8294	0	HOH	536	15.652	-33.654	161.052	1.00 39.31		0
	MOTA	8295	0	HOH	537		-73.270		1.00 52.60		0
10	MOTA	8296	0	HOH	538		-96.434		1.00 51.75		0
	MOTA	8297	0	HOH	539		-47.480	169.785	1.00 42.26		0
	MOTA	8298	0	нон	540		-40.089		1.00 44.31		0
	MOTA	8299	0	HOH	542		-99.754	106.625	1.00 42.46		0
4.5	MOTA	8300	0	нон	543		-59.003		1.00 38.14		0
15	MOTA	8301	0	НОН	544		-39.031		1.00 43.59		0
	MOTA	8302	0	нон	545		-14.277		1.00 51.26		0
	ATOM	8303	0	НОН	546		-97.785		1.00 39.90		0
	ATOM	8304	0	нон	547		-98.465		1.00 48.51		0
20	MOTA	8305	0	нон	548			122.376	1.00 47.73		0
20	MOTA	8306	0	нон	549			107.995	1.00 26.18	S	0
	ATOM	8307	0	нон	551			170.747	1.00 34.90	S	0
	ATOM	8308	0	нон	552			105.920	1.00 50.86	S	0
	ATOM	8309	0	нон	553			145.088	1.00 55.30	S	0
25	ATOM	8310	0	нон	554			149.518 147.215	1.00 43.14	S	0
23	ATOM ATOM	8311 8312	0	НОН НОН	555 557	_	-33.662		1.00 44.48 1.00 39.72	S S	0
	ATOM	8313	0	нон	557 558			152.237	1.00 39.72	S	0
	ATOM	8314	0	нон	559		-67.927		1.00 42.78	S	0
	MOTA	8315	ŏ	нон	560			168.443	1.00 42.48	S	0
30	ATOM	8316	Ö	нон	561			115.196	1.00 68.97	S	o
00	ATOM	8317	ŏ	нон	562		-66.758		1.00 58.70	S	ŏ
	ATOM	8318	ŏ	нон	563		-71.240		1.00 47.55	s	ŏ
	ATOM	8319	ō	нон	564		-90.428		1.00 40.50	s	ō
	ATOM	8320	ō	нон	565		-37.312		1.00 45.44	S	ō
35	MOTA	8321	Ō	НОН	566		-96.445		1.00 46.91	s	Ō
	MOTA	8322	0	нон	567		-34.354		1.00 38.19	S	O
	MOTA	8323	0	нон	568	-6.686			1.00 40.62	S	0
	MOTA	8324	0	нон	569	0.603	-92.714		1.00 49.80	S	0
	ATOM	8325	0	HOH	570	-10.908	-44.492	149.043	1.00 55.75	S	0
40	ATOM	8326	0	HOH	571	11.715	-56.940	144.398	1.00 50.46	S	0
	MOTA	8327	0	HOH	575			110.121	1.00 77.11	S	0
	MOTA	8328	0	нон	576			104.387	1.00 50.00	S	0
	MOTA	8329	0	HOH	577			121.036	1.00 48.12	S	0
	MOTA	8330	0	HOH	578			108.101	1.00 41.31	S	0
45	MOTA	8331	0	HOH	580			170.420	1.00 47.84	S	0
	MOTA	8332	0	HOH	583			147.872	1.00 46.19	S	0
	MOTA	8333	0	нон	584		-38.154		1.00 52.49	S	0
	MOTA	8334	0	HOH	585			118.436	1.00 43.61	S	0
50	MOTA	8335	0	нон	586			147.950	1.00 49.22	S	0
50	MOTA	8336		НОН	587			151.620	1.00 48.37	S	0
	ATOM	8337		нон	590			5 151.484	1.00 54.81	S	0
	ATOM	8338		нон	591			136.375	1.00 39.42	S	0
	ATOM	8339		нон	592		-44.413		1.00 55.03	S	0
55	ATOM	8340		нон	593			5 150.116	1.00 51.39	S	0
55	ATOM	8341		нон	594			154.053	1.00 44.25	S	0
	ATOM	8342		нон	595 507			7 169.236	1.00 53.46	s s	0
	ATOM	8343		HOH	597 509			2 136.494	1.00 41.41	S	0
	MOTA	8344	0	нон	598	-4.024	· -30./6	5 138.695	1.00 54.76	S	0

-313-

	MOTA	8345	0	HOH	599		-13.288		1.00 41.25		0
	MOTA	8346	0	HOH	601	-10.913			1.00 50.93		0
	ATOM	8347	0	HOH	603		-24.982		1.00 47.50		0
_	MOTA	8348	0	нон	604		-94.049		1.00 42.28		0
5	MOTA	8349	0	нон	605	-14.289			1.00 52.11		0
	MOTA	8350	0	НОН	606	-19.924		99.672	1.00 57.18	S	0
	MOTA	8351	0	НОН	607		-35.468		1.00 46.97	S	0
	MOTA	8352	0	нон	608		-94.614		1.00 40.46	S	0
40	MOTA	8353	0	нон	609			107.395	1.00 55.14	S	0
10	MOTA	8354	0	нон	610			116.432	1.00 37.22	S	0
	MOTA	8355	0	нон	611	-10.377			1.00 44.74	S	0
	MOTA	8356	0	нон	612			133.659	1.00 45.83	S	0
	MOTA	8357	0	HOH	614	-12.440			1.00 34.32	S	0
4-	MOTA	8358	0	нон	617			112.739	1.00 50.67	S	0
15	MOTA	8359	0	нон	618			169.501	1.00 48.06	S	0
	ATOM	8360	0	HOH	619			148.628	1.00 54.49	S	0
	MOTA	8361	0	HOH	620			136.844	1.00 53.29	S	0
	MOTA	8362	0	нон	621			164.880	1.00 46.75	S	0
	MOTA	8363	0	HOH	623			148.740	1.00 58.12	S	0
20	MOTA	8364	0	HOH	626			146.410	1.00 52.87	S	0
	MOTA	8365	0	HOH	627			128.206	1.00 61.98	S	0
	MOTA	8366	0	HOH	628			170.673	1.00 41.69	S	0
	MOTA	8367	0	HOH	629			155.302	1.00 39.69	S	0
	MOTA	8368	0	HOH	630			116.783	1.00 48.41	S	0
25	MOTA	8369	0	HOH	631			165.191	1.00 46.58	S	0
	MOTA	8370	0	HOH	633			169.718	1.00 41.32	S	0
	ATOM	8371	0	HOH	634			111.912	1.00 48.12	S	0
	MOTA	8372	0	нон	635		-57.565		1.00 32.16	S	0
00	MOTA	8373	0	НОН	636			147.829	1.00 42.76	S	0
30	MOTA	8374	0	HOH	637			122.015	1.00 37.58	S	0
	ATOM	8375	0	HOH	638			152.992	1.00 55.36	S	0
	ATOM	8376	0	нон	639			108.941	1.00 40.46	S	0
	MOTA	8377	0	нон	640		-31.755		1.00 55.93	S	0
00	MOTA	8378	0	HOH	641			104.096	1.00 48.46	S	0
35	MOTA	8379	0	HOH	642			150.732	1.00 50.86	S	0
	MOTA	8380	0	HOH	643			123.781	1.00 49.25	S	0
	MOTA	8381	0	HOH	644			103.761	1.00 53.33	S	0
	MOTA	8382	0	нон	645			166.992	1.00 59.33	S	0
40	MOTA	8383	0	нон	646			169.143	1.00 50.88	S	0
40	MOTA	8384	0	нон	647			141.775	1.00 62.45	S	0
	MOTA	8385	0	HOH	648			141.840	1.00 53.76	S	0
	ATOM	8386	0	нон	649			101.833	1.00 51.97	S	0
	MOTA	8387	0	нон	651			147.662	1.00 44.65	S	0
45	MOTA	8388	0	нон	653			3 134.022	1.00 53.05	S	0
45	ATOM	8389	0	нон	655			138.891	1.00 54.56	S	0
	ATOM	8390	0	НОН	656			5 121.208	1.00 50.84	S	0
	MOTA	8391	0	нон	658			144.738	1.00 47.88	S	0
	MOTA	8392		НОН	659			110.573	1.00 41.41	s	0
50	MOTA	8393		нон	661			1 102.774	1.00 47.84	S	0
50	MOTA	8394		нон	663		-75.062		1.00 52.90	S	0
	MOTA	8395		нон	664			7 101.333	1.00 57.41	S	0
	MOTA	8396		нон	668			B 170.230	1.00 51.20	S	0
	MOTA	8397		НОН	672			0 160.931	1.00 52.16	S	0
EE	ATOM	8398		НОН	673			1 106.971	1.00 62.83	S	0
55	MOTA	8399		нон	674			3 106.975	1.00 43.13	S	0
	MOTA	8400		нон	676			1 110.887	1.00 43.22	S	0
	MOTA	8401			677			1 104.475		S	0
	MOTA	8402	0	нон	681	-10.652	2 -35.07	5 160.241	1.00 52.13	S	0

-314-

	MOTA	8403	0	HOH	685		-82.942		1.00 54.94	S	0
	MOTA	8404	0	нон	686	-12.713			1.00 70.33	S	0
	MOTA	8405	0	нон	689	-10.374			1.00 55.51	S	0
_	MOTA	8406	0	НОН	690	-15.464			1.00 50.64	S	0
5	MOTA	8407	0	НОН	691		-60.842		1.00 68.98	S	0
	MOTA	8408	0	НОН	692		-44.563		1.00 52.71	S	0
	MOTA	8409	0	НОН	693		-94.906		1.00 42.37	S	0
	MOTA	8410	0	нон	695		-62.997		1.00 43.89	S	0
40	MOTA	8411	0	НОН	697		-62.955		1.00 67.72	S	0
10	MOTA	8412	0	HOH	698		-84.834	96.026	1.00 68.94	S	0
	ATOM	8413	0	нон	701	-19.964			1.00 70.97	S	0
	MOTA	8414	0	нон	702	-17.043			1.00 52.11	S	0
	MOTA	8415	0	HOH	703		-29.599		1.00 44.42	S	0
	MOTA	8416	0	HOH	708	-13.381		97.616	1.00 54.25	S	0
15	MOTA	8417	0	HOH	709			158.139	1.00 55.23	S	0
	MOTA	8418	0	HOH	714			158.773	1.00 43.63	S	0
	ATOM	8419	0	HOH	719	-2.397	-85.569	126.958	1.00 51.95	S	0
	ATOM	8420	0	HOH	723			117.416	1.00 57.09	S	0
	ATOM	8421	0	HOH	725	-20.095	-93.695	156.379	1.00 48.48	S	0
20	MOTA	8422	0	HOH	728	-20.097	-34.574	98.029	1.00 45.93	S	0
	MOTA	8423	0	HOH	730	5.820	-62.677	172.241	1.00 52.85	S	0
	ATOM	8424	0	HOH	733	14.590	-77.427	94.470	1.00 48.88	S	0
	MOTA	8425	0	HOH	734	-9.869	-22.276	134.367	1.00 72.16	S	0
	ATOM	8426	0	HOH	735	5.303	-36.085	129.231	1.00 30.02	S	0
25	MOTA	8427	0	HOH	736	3.098	-34.827	125.987	1.00 26.22	S	0
	ATOM	8428	0	HOH	737	10.874	-90.931	100.638	1.00 41.15	S	0
	ATOM	8429	0	нон	738	-23.151	-61.565	160.742	1.00 32.42	S	0
	ATOM	8430	0	нон	739	-8.831	-59.000	93.865	1.00 32.91	S	0
	ATOM	8431	0	нон	741			150.140	1.00 25.10	S	0
30	MOTA	8432	0	нон	742			155.807	1.00 40.46	S	0
	ATOM	8433	Ō	нон	743			105.014	1.00 40.07	S	0
	ATOM	8434	0	нон	744			105.086	1.00 29.75	S	0
	ATOM	8435	ō	нон	745			144.159	1.00 34.27	S	0
	MOTA	8436	ō	нон	746			105.752	1.00 34.90	S	0
35	ATOM	8437	ō	нон	747			162.206	1.00 31.38	s	0
- •	ATOM	8438	ō	НОН	748			107.364	1.00 43.45	S	0
	ATOM	8439	ŏ	нон	749		-39.637		1.00 60.23	S	Ō
	ATOM	8440	ō	нон	750			157.176	1.00 35.25	s	Ō
	ATOM	8441	ŏ	нон	751			130.416	1.00 51.18	S	ō
40	ATOM	8442	ŏ	нон	756			135.708	1.00 70.13	s	ō
	ATOM	8443	ŏ	нон	760			154.565	1.00 51.07	S	ō
	ATOM	8444	ŏ	нон	768			123.786	1.00 58.62	S	ō
	ATOM	8445	ŏ	нон	770			7 135.470	1.00 48.19	S	ō
	ATOM	8446	ő	нон	771			3 168.175	1.00 49.12	s	Ö
45	ATOM	8447	Ö	нон	773			105.507	1.00 49.76	s	Ö
70	ATOM	8448		нон	774			5 101.201	1.00 56.64	s	ŏ
		8449		нон	775			115.724	1.00 55.57	s	ŏ
	MOTA	8450		нон	776		-49.262		1.00 33.00	s	Ö
	ATOM	8451		нон	777			5 160.148	1.00 54.59	Š	ŏ
50	ATOM				778			4 160.150	1.00 47.65	s	ŏ
30	ATOM	8452		HOH				6 151.229	1.00 42.84	S	0
	MOTA	8453		HOH	779 783			6 106.538	1.00 42.84	S	0
	ATOM	8454		нон							
	MOTA	8455		нон	784			0 125.976			
EE	ATOM	8456		НОН	785			8 129.815			
55	MOTA	8457		нон	786			7 129.222			
	ATOM	8458		нон	787			0 134.871			
	MOTA	8459		нон	788			8 159.140			
	MOTA	8460	0	HOH	789	11.18	, -59.27	3 158.430	1.00 33.45	S	0

-315-

		0461	_		700	15 700	26 010	152	E 0.0	1 00	36.09	s	0
	ATOM	8461	0	НОН	790	-15.720					44.35		Ö
	ATOM	8462	0	нон	791		-32.487						
	MOTA	8463	0	нон	795		-86.248				37.18		0
_	MOTA	8464	0	НОН	802		-43.210				61.28		0
5	MOTA	8465	0	НОН	804		-52.04		549		27.57		0
	MOTA	8466	0	нон	805		-36.88				39.77		0
	MOTA	8467	0	HOH	806		-46.69				45.60		0
	MOTA	8468	0	HOH	807	-14.220					27.66	S	0
	MOTA	8469	0	нон	808	-10.216	-54.37	6 157.	. 359	1.00	36.07	S	0
10	TER	8470		HOH	808							S	
	MOTA	8471	C1	596	1		-45.92				18.61	L	C
	MOTA	8472	N2	596	1	-2.499	-44.80	5 105	.931	1.00	19.75	L.	N
	MOTA	8473	C3	596	1		-45.71			1.00	19.36	L	C
	MOTA	8474	C4	596	1		-47.09			1.00	19.46	L	C
15	MOTA	8475	C5	596	1	-1.505	-44.00	3 106	.355	1.00	20.57	L	С
	ATOM	8476	C6	596	1	-3.571	-44.49	5 104	. 958	1.00	18.69	L	C
	MOTA	8477	N7	596	1	-0.807	-44.50	1 107	.372	1.00	19.90	L	N
	MOTA	8478	C8	596	1	-1.092	-46.66	9 108	.636	1.00	18.27	L	C
	MOTA	8479	C9	596	1		-48.09			1.00	19.94	L	С
20	ATOM	8480		596	1		-42.68			1.00	22.09	L	N
	ATOM	8481		596	1	-4.572	-43.44	1 105	.486	1.00	18.66	L	С
	MOTA	8482		596	1		-47.85				19.06	L	С
	ATOM	8483		596	1		-49.31				20.54	L	С
	ATOM	8484		596	1		-41.76				23.52	L	С
25	ATOM	8485		596	1		-43.94				18.98	L	C
	ATOM	8486		596	1		-49.32			1.00	20.47	L	N
	ATOM	8487		596	ī		-50.27		_		21.54	L	0
	ATOM	8488		596	1		-40.38				23.09	L	С
	ATOM	8489		596	1		-41.95				23.60	L	C
30	MOTA	8490		596	ī		-43.72				19.73	L	C
•	MOTA	8491		596	ī		-44.73				18.94	L	Č
	ATOM	8492		596	ī		-40.12				23.10	L	Č
	ATOM	8493		596	1		-39.35				23.56	L	Č
	MOTA	8494		596	ī		-42.89				23.72	L	C
35	ATOM	8495		596	1		-41.17				23.90	L	C
•	ATOM	8496		596	ī		-44.39				20.03	L	Č
	ATOM	8497		596	1		-45.34				19.94	L	Č
	ATOM	8498		596	1		-38.9				23.17	L	Č
	ATOM	8499		596	ĩ		4 -38.1				23.29	L	Č
40	ATOM	8500		596	1		2 -43.0				24.28	L	Č
	ATOM	8501		596	î		0 -41.2				24.30	L	Č
	ATOM	8502		2 596	ī		6 -45.1				19.58	L	Ċ
	MOTA	8503		3 596	1		4 -37.9				23.09	L	Ċ
	MOTA	8504		1 596	1		6 -42.1				23.94	L	Č
45	MOTA	8505		5 596	î		1 -47.2				19.63	L	н
-10	ATOM	8506		5 596	ī		0 -45.3				0 19.04	L	Н
	ATOM	8507		7 596	î		0 -44.1				19.09	L	Н
	ATOM	8508		8 596	1		5 -46.5				0 18.86	L	H
	ATOM	8509		9 596	ī		2 -42.3				0 22.39	L	H
50	ATOM	8510		0 596	ī		8 -43.1				0 18.82	L	н
00				1 596	ī		0 -42.5				0 18.85	L	H
	MOTA	8511 8512		2 596	1		4 - 48.5				0 10.03		Н
	MOTA			3 596	1		4 -40.5 3 -41.9				0 23.34		H
	MOTA	8513		3 596 4 596	1		3 -41.5 3 -48.5				0 23.34		Н
55	MOTA	8514			1		3 -40.3 3 -50.1				0 20.73		Н
55	MOTA	8515		5 596			1 -43.1				0 20.71		Н
	MOTA	8516		6 596	1		4 -44.9				0 19.30		Н
	ATOM	8517		7 596	1						0 13.30		H
	MOTA	8518	H4	8 596	1	-2.21	7 -40.8	J, 10	,	1.0	U 2J.ZI	ם	п

-316-

	ATOM	8519	H49		1		-39.503		1.00 23.37	L	H
	MOTA	8520	H50	596	1	0.781	-43.548	104.470	1.00 23.80	L	H
	MOTA	8521	H51	596	1	2.062	-40.480	107.234	1.00 23.82	L	н
	ATOM	8522	H52	596	1	-5.160	-44.208	110.074	1.00 19.98	L	Н
5	ATOM	8523	H53	596	1	-8.005	-45.966	107.398	1.00 19.79	L	H
	ATOM	8524	H54	596	1	-3.517	-38.756	107.729	1.00 23.18	L	H
	MOTA	8525	H55	596	1		-37.365		1.00 23.37	L	Н
	ATOM	8526	H56	596	1		-43.752		1.00 24.22	L	н
	ATOM	8527	H57		ī		-40.656		1.00 24.15	L	Н
10	ATOM	8528	н58	596	ī		-45.633		1.00 19.69	L	H
	ATOM	8529	н59		1		-36.980		1.00 23.46	L	H
	ATOM	8530	H60		î		-42.244		1.00 23.40		н
	ATOM	8531	C1	596	2					L	
							-69.170		1.00 17.81	R	C
45	ATOM	8532	N2	596	2		-70.327		1.00 17.06	R	N
15	MOTA	8533	C3	596	2		-69.331		1.00 18.16	R	C
	ATOM	8534	C4	596	2			107.183	1.00 17.87	R	С
	MOTA	8535	C5	596	2			106.552	1.00 17.68	R	С
	MOTA	8536	C6	596	2			105.341	1.00 16.75	R	С
	MOTA	8537	N7	596	2			107.475	1.00 18.02	R	N
20	ATOM	8538	C8	596	2	2.820	-68.344	108.702	1.00 17.84	R	C
	MOTA	8539	C9	596	2	4.789	-67.013	108.148	1.00 18.61	R	С
	ATOM	8540	N10	596	2	3.123	-72.420	106.004	1.00 18.38	R	N
	MOTA	8541	C11	596	2	6.546	-71.662	105.985	1.00 16.15	R	C
	ATOM	8542	C12	596	2	3.605	-67.184	108.904	1.00 17.98	R	C
25	MOTA	8543		596	2			108.504	1.00 18.62	R	C
	ATOM	8544		596	2			106.474	1.00 18.34	R	Ċ
	ATOM	8545		596	2			107.206	1.00 16.15	R	č
	ATOM	8546		596	2			108.153	1.00 18.90	R	N
	ATOM	8547		596	2			109.159	1.00 20.09	R	ő
30	ATOM	8548		596	2			106.388	1.00 20.03	R	c
00	ATOM	8549	-	596	2			105.780	1.00 17.44	R	C
		8550		596	2			103.780			
	ATOM								1.00 16.48	R	C
	ATOM	8551		596	2			107.048	1.00 15.06	R	C
35	ATOM	8552		596	2			107.305	1.00 16.86	R	C
33	MOTA	8553		596	2			105.424	1.00 17.31	R	С
	MOTA	8554		596	2			104.758	1.00 19.86	R	C
	MOTA	8555		596	2			106.157	1.00 21.14	R	С
	MOTA	8556		596	2			109.617	1.00 16.65	R	C
40	MOTA	8557		596	2			108.142	1.00 15.10	R	С
40	ATOM	8558		596	2			107.242	1.00 16.83	R	С
	MOTA	8559	C29	596	2	3.005	-76.891	105.375	1.00 17.45	R	C
	ATOM	8560	C30	596	2	-0.709	-71.956	104.108	1.00 21.12	R	C
	MOTA	8561	C31	596	2	-1.677	-73.701	105.487	1.00 22.11	R	С
	MOTA	8562	C32	596	2	8.415	-69.847	109.421	1.00 16.40	R	С
45	ATOM	8563	C33	596	2	4.039	-77.149	106.291	1.00 17.12	R	C
	ATOM	8564	C34	596	2	-1.801	-72.758	104.454	1.00 21.79	R	С
	ATOM	8565		596	2	6.024	-67.954	106.594	1.00 18.11	R	Н
	ATOM	8566		596	2			105.110	1.00 16.89	R	Н
	ATOM	8567		596	2			104.403	1.00 16.85	R	
50	ATOM	8568		596	2			109.299	1.00 18.19	R	
•	MOTA	8569		596	2			105.274	1.00 18.51	R	
	ATOM	8570		596	2			105.252	1.00 16.39	R	
				596	2			105.232	1.00 16.39	R	
	MOTA	8571									
55	MOTA	8572		596	2			109.657		R	_
J	MOTA	8573		596	2			107.522		R	
	ATOM	8574		596	2			107.652		R	
	MOTA	8575		596	2			108.408		R	
	ATOM	8576	H46	596	2	5.903	-72.034	1 108.633	1.00 16.43	R	Н

-317-

	MOTA	8577	H47 596	2	8.758	-70.133	106.057	1.00 15.62	R	H
	MOTA	8578	H48 596	2	3.925	-74.260	108.081	1.00 16.88	R	H
	MOTA	8579	H49 596	2	1.556	-75.498	104.697	1.00 17.51	R	H
_	MOTA	8580	H50 596	2	1.310	-71.479	104.438	1.00 20.27	R	Н
5	ATOM	8581	H51 596	2	-0.390	-74.586	106.951	1.00 21.25	R	Н
	ATOM	8582	H52 596	2	6.891	-70.827	110.605	1.00 16.51	R	Н
	MOTA	8583	H53 596	2	9.797	-69.006	108.010	1.00 15.29	R	Н
	MOTA	8584	H54 596	2	5.161	-76.405	107.946	1.00 17.12	R	H
	ATOM	8585	н55 596	2	2.723	-77.634	104.647	1.00 17.47	R	H
10	ATOM	8586	н56 596	2	-0.806	-71.205	103.339	1.00 21.25	R	Н
	MOTA	8587	H57 596	2	-2.512	-74.336	105.751	1.00 22.07	R	H
	ATOM	8588	H58 596	2	8.852	-69.329	110.259	1.00 16.27	R	Н
	ATOM	8589	н59 596	2	4.558	-78.095	106.287	1.00 17.47	R	Н
	MOTA	8590	H60 596	2	-2.735	-72.657	103.923	1.00 21.89	R	Н
15	MOTA	8591	C1 596	3	2.846	-46.116	157.632	1.00 15.32	T	С
	ATOM	8592	N2 596	3	2.939	-44.983	158.430	1.00 16.26	T	N
	ATOM	8593	C3 596	3	1.752	-45.890	156.704	1.00 15.57	T	С
	ATOM	8594	C4 596	3	3.601	-47.287	157.515	1.00 14.61	${f T}$	C
	ATOM	8595	C5 596	3	1.945	-44.165	157.987	1.00 16.95	T	C
20	ATOM	8596	C6 596	3	4.027	-44.670	159.405	1.00 15.77	T	C
	ATOM	8597	ท7 596	3	1.214	-44.671	156.986	1.00 14.76	\mathbf{T}	N
	ATOM	8598	C8 596	3	1.501	-46.839	155.702	1.00 14.30	\mathbf{T}	C
	MOTA	8599	C9 596	3	3.340	-48.270	156.482	1.00 15.09	T	С
	ATOM	8600	N10 596	3	1.720	-42.818	158.524	1.00 16.85	T	N
25	ATOM	8601	C11 596	3	5.028	-43.656	158.829	1.00 15.65	T	С
	ATOM	8602	C12 596	3			155.565	1.00 14.20	${f T}$	C
	ATOM	8603	C13 596	3	4.091	-49.540	156.364	1.00 13.71	${f T}$	С
	ATOM	8604	C14 596	3	0.792	-41.854	157.922	1.00 16.81	\mathbf{T}	C
	ATOM	8605	C15 596	3	5.841	-44.235	157.706	1.00 16.86	T	C
30	MOTA	8606	N16 596	3			156.931	1.00 12.82	T	N
	ATOM	8607	017 596	3			155.803	1.00 12.64	T	0
	ATOM	8608	C18 596	3			157.929	1.00 15.58	T	C
	MOTA	8609	C19 596	3	-0.633	-41.901	158.482	1.00 16.81	T	С
	MOTA	8610	C20 596	3			156.366	1.00 17.32	\mathbf{T}	C
35	ATOM	8611	C21 596	3	6.943	-45.071	157.971	1.00 17.36	T	C
	ATOM	8612	C22 596	3	2.526	-40.356	156.970	1.00 15.60	\mathbf{T}	С
	MOTA	8613	C23 596	3	1.327	-39.508	158.869	1.00 15.97	T	C
	ATOM	8614	C24 596	3	-1.027	-42.802	159.499	1.00 17.21	T	C
	ATOM	8615	C25 596	3	-1.623	-41.014	157.976	1.00 17.34	T	С
40	ATOM	8616	C26 596	3	6.087	-44.738	155.318	1.00 17.94	T	С
	MOTA	8617	C27 596	3			156.911	1.00 18.26	T	C
	MOTA	8618	C28 596	3	3.327	-39.207	156.961	1.00 15.61	\mathbf{T}	С
	MOTA	8619		3	2.072	-38.320	158.836	1.00 16.06	T	С
	MOTA	8620		3	-2.333	-42.774	160.051	1.00 17.06	T	С
45	MOTA	8621	C31 596	3	-2.922	-40.988	158.511	1.00 17.58	T	C
	ATOM	8622		3	7.181	-45.565	155.595	1.00 17.92	T	С
	ATOM	8623		3	3.089	-38.180	157.872	1.00 15.78	T	С
	MOTA	8624		3	-3.260	-41.857	159.552	1.00 17.41	T	C
	MOTA	8625		3	4.396	-47.438	158.229	1.00 14.89	T	Н
50	ATOM	8626		3	4.548	-45.560	159.719	1.00 16.02	T	Н
	ATOM	8627		3			3 160.303	1.00 16.08	T	
	ATOM	8628		3			5 154.998	1.00 14.65	T	Н
	ATOM	8629		3	2.263	-42.518	3 159.303	1.00 17.20	T	
	ATOM	8630		3			159.607		T	
55	ATOM	8631		3			7 158.496		T	
	ATOM	8632		3			1 154.791		T	
	ATOM	8633		3			2 156.879		T	
	ATOM	8634		3			2 157.389		T	

-318-

	MOTA	8635	H45 596	3	5.897	-50.359	156.902	1.00 12.70	T	Н
	MOTA	8636	H46 596	3	4.608	-43.403	156.149	1.00 17.56	T	Н
	MOTA	8637	H47 596	3		-45.259		1.00 17.47	T	Н
	ATOM	8638	H48 596	3		-41.118		1.00 15.78	T	Н
5	MOTA	8639	H49 596			-39.633		1.00 16.06	T	Н
	ATOM	8640	H50 596			-43.510		1.00 17.16	Ť	н
	ATOM	8641	H51 596			-40.340		1.00 17.10		
	ATOM	8642	H52 596			-44.629			T	Н
	ATOM	8643	H53 596					1.00 17.79	T	Н
10	ATOM	8644				-46.371		1.00 18.15	T	Н
10			H54 596			-39.108		1.00 15.83	T	Н
	ATOM	8645	H55 596			-37.532		1.00 15.79	T	Н
	MOTA	8646	H56 596			-43.416		1.00 17.05	T	Н
	MOTA	8647	H57 596			-40.295		1.00 17.59	${f T}$	Н
45	MOTA	8648	H58 596			-46.063		1.00 18.12	T	Н
15	MOTA	8649	H59 596			-37.276		1.00 15.95	T	H
	MOTA	8650	H60 596		-4.247	-41.800	159.990	1.00 17.61	\mathbf{T}	H
	MOTA	8651	C1 596	4	-5.000	-68.974	157.356	1.00 15.41	V	C
	MOTA	8652	N2 596	4	-5.233	-70.123	158.103	1.00 15.55	V	N
	MOTA	8653	C3 596	4	-3.819	-69.217	156.559	1.00 16.29	V	C
20	ATOM	8654	C4 596	4		-67.768		1.00 15.23	v	C
	ATOM	8655	C5 596			-70.970		1.00 17.80	v	Č
	MOTA	8656	C6 596	4		-70.373		1.00 14.78	v	č
	MOTA	8657	N7 596			-70.481		1.00 17.03	v	N
	ATOM	8658	C8 596			-68.243		1.00 17.05	v	C
25	MOTA	8659	C9 596			-66.775		1.00 15.00	v	C
	ATOM	8660	N10 596			-72.308		1.00 10.10		
	ATOM	8661	C11 596			-72.308			V	N
	ATOM	8662	C12 596					1.00 15.05	V	C
	ATOM	8663				-67.015		1.00 15.69	V	C
30						-65.520		1.00 15.40	V	С
50	ATOM	8664	C14 596			-73.285		1.00 20.54	V	C
	ATOM	8665	C15 596			-70.681		1.00 14.31	V	C
	ATOM	8666	N16 596			-65.478		1.00 15.48	V	N
	MOTA	8667	017 596			-64.575		1.00 16.46	V	0
25	MOTA	8668	C18 596			74.624		1.00 20.15	V	C
35	ATOM	8669	C19 596			-73.205		1.00 21.79	V	C
	MOTA	8670	C20 59			-70.955		1.00 14.50	V	C
	ATOM	8671	C21 596	5 4		-69.808		1.00 13.56	V	C
	ATOM	8672	C22 59	5 4	-4.843	-74.838	156.878	1.00 19.47	V	C
	ATOM	8673	C23 596	5 4	-3.638	-75.621	158.809	1.00 20.11	V	C
40	ATOM	8674	C24 596	5 4	-1.491	-72.278	159.483	1.00 22.05	v	C
	ATOM	8675	C25 59	5 4		-74.027		1.00 22.52	v	Č
	MOTA	8676	C26 59	5 4		-70.297		1.00 15.23	V	
	ATOM	8677	C27 59	5 4		-69.180		1.00 14.11	V	C
	MOTA	8678	C28 59			-76.022		1.00 20.11	v	č
45	ATOM	8679	C29 59			76.816		1.00 19.91	v	C
	ATOM	8680	C30 59			-72.173		1.00 22.72	v	C
	ATOM	8681	C31 59		_	73.914		1.00 23.89	v	
	ATOM	8682	C32 59				154.798	1.00 23.89		C
	ATOM	8683	C33 59				157.857		V	C
50								1.00 19.08	V	C
	ATOM	8684	C34 59			-72.998		1.00 23.31	V	C
	MOTA	8685	H35 59				157.776	1.00 15.39	V	Н
	MOTA	8686	H36 59				159.250	1.00 15.16	V	H
	MOTA	8687	H37 59				159.890	1.00 15.23	V	H
66	ATOM	8688	H38 59				155.105	1.00 15.91	V	H
55	MOTA	8689	н39 59				158.987	1.00 19.56	V	H
	ATOM	8690	H40 59				159.057	1.00 14.81	V	H
	ATOM	8691	H41 59				158.063		V	H
	MOTA	8692	H42 59	6 4	-3.664	4 -66.262	154.828	1.00 16.36	V	H

-319-

	MOTA	8693	H43	596	4	-3.023	-73.063	156.736	1.00	20.49	V	H
	MOTA	8694	H44	596	4	-7.674	-66.265	156.678	1.00	15.81	V	H
	MOTA	8695	H45	596	4	-7.746	-64.660	156.003	1.00	15.79	V	H
	MOTA	8696	H46	596	4	-6.745	-71.667	155.781	1.00	14.88	V	H
5	ATOM	8697	H47	596	4	-9.601	-69.601	158.167	1.00	14.04	V	H
	MOTA	8698	H48	596	4	-5.019	-74.086	156.124	1.00	19.70	V	Н
	ATOM	8699	H49	596	4	-2.932	-75.479	159.612	1.00	20.34	V	Н
	MOTA	8700	H50	596	4	-2.242	-71.633	159.911	1.00	22.23	V	Н
	MOTA	8701	H51	596	4	-0.914	-74.727	157.153	1.00	22.61	V	Н
10	MOTA	8702	H52	596	4	-7.560	-70.482	153.747	1.00	15.36	V	Н
	MOTA	8703	H53	596	4	-10.538	-68.503	156.125	1.00	14.26	V	H
	MOTA	8704	H54	596	4	-6.380	-76.155	156.163	1.00	19.84	V	H
	MOTA	8705	H55	596	4	-4.177	-77.575	159.533	1.00	20.19	V	H
	ATOM	8706	H56	596	4	-0.042	-71.464	160.825	1.00	23.01	V	H
15	ATOM	8707	H57	596	4	1.346	-74.536	158.135	1.00	23.57	V	Н
	ATOM	8708	H58	596	4	-9.501	-68.923	153.917	1.00	14.82	V	H
	MOTA	8709	H59	596	4	-5.939	-77.923	157.887	1.00	19.84	V	Н
	ATOM	8710	H60	596	4	1.775	-72.930	160.006	1.00	23.48	V	Н

-320-

References

The references listed below as well as all references cited in the specification are incorporated herein by reference to the extent that they supplement, explain, provide a background for or teach methodology, techniques and/or compositions employed herein.

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PCT/US2004/023092

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It will be understood that various details of the invention can be changed without departing from the scope of the invention. Furthermore, the foregoing description is for the purpose of illustration only, and not for the purpose of limitation, the invention being defined by the claims.